



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 7, 2023 – 09:29 AM EST

PDB ID : 5J3C  
Title : Thermus thermophilus 70S termination complex containing E. coli RF1  
Authors : Hoffer, E.D.; Dunham, C.M.  
Deposited on : 2016-03-30  
Resolution : 3.04 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : **FAILED**  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

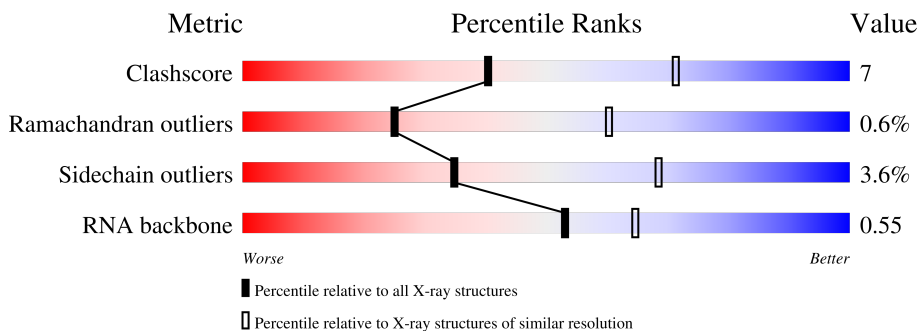
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.04 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	3096 (3.08-3.00)
Ramachandran outliers	138981	2986 (3.08-3.00)
Sidechain outliers	138945	2988 (3.08-3.00)
RNA backbone	3102	1034 (3.30-2.78)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	RA	2915	
1	YA	2915	
2	RB	122	
2	YB	122	
3	RD	276	
3	YD	276	

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Mol	Chain	Length	Quality of chain
4	RE	206	77% 20% ..
4	YE	206	76% 21% ..
5	RF	210	73% 21% ..
5	YF	210	69% 27% ..
6	RG	182	75% 25% .
6	YG	182	71% 25% ..
7	RH	180	82% 14% ..
7	YH	180	68% 28% ..
8	RI	148	80% 18% ..
8	YI	148	80% 15% ..
9	RN	140	81% 17% .
9	YN	140	83% 14% .
10	RO	122	76% 24%
10	YO	122	81% 18% .
11	RP	150	78% 19% ..
11	YP	150	75% 21% ..
12	RQ	141	81% 18% .
12	YQ	141	77% 21% .
13	RR	118	75% 22% .
13	YR	118	81% 19%
14	RS	112	80% 15% ..
14	YS	112	81% 16% ..
15	RT	146	66% 20% . 10%
15	YT	146	71% 17% . 10%
16	RU	118	81% 16% ..









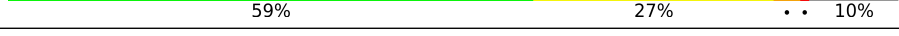

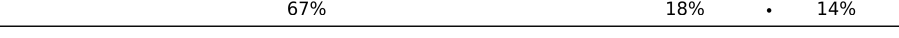
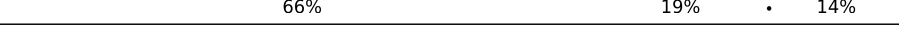

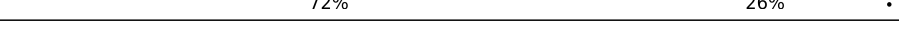


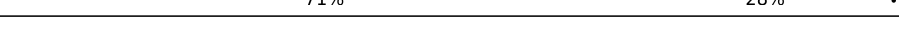

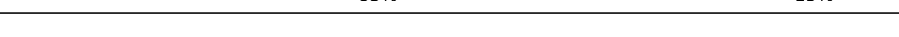






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Mol	Chain	Length	Quality of chain
16	YU	118	83% 15% .
17	RV	101	83% 15% .
17	YV	101	79% 19% ..
18	RW	113	84% 14% ..
18	YW	113	81% 18% ..
19	RX	96	76% 23% .
19	YX	96	88% 11% .
20	RY	110	76% 20% ..
20	YY	110	75% 21% ..
21	RZ	206	83% 14% ..
21	YZ	206	85% 12% .
22	R0	85	74% 14% . 9%
22	Y0	85	73% 16% . 9%
23	R1	98	81% 17% ..
23	Y1	98	76% 21% ..
24	R2	72	75% 22% .
24	Y2	72	79% 18% .
25	R3	60	87% 12% .
25	Y3	60	78% 18% ..
26	R4	71	58% 35% ...
26	Y4	71	63% 30% ...
27	R5	60	73% 22% ..
27	Y5	60	83% 13% ..
28	R6	54	76% 22% .
28	Y6	54	80% 19% .

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Mol	Chain	Length	Quality of chain
29	R7	49	 71% 27%
29	Y7	49	 69% 29%
30	R8	65	 72% 23%
30	Y8	65	 69% 29%
31	R9	37	 59% 41%
31	Y9	37	 68% 32%
32	QA	1521	 60% 32% 6%
32	XA	1521	 60% 32% 6%
33	QB	256	 59% 27% 10%
33	XB	256	 55% 30% 5% 10%
34	QC	239	 67% 18% 14%
34	XC	239	 66% 19% 14%
35	QD	209	 64% 34%
35	XD	209	 72% 26%
36	QE	162	 65% 26% 9%
36	XE	162	 69% 22% 9%
37	QF	101	 71% 28%
37	XF	101	 86% 12%
38	QG	156	 83% 15%
38	XG	156	 83% 15%
39	QH	138	 78% 21%
39	XH	138	 78% 21%
40	QI	128	 68% 29%
40	XI	128	 62% 34%
41	QJ	105	 57% 33% 8%




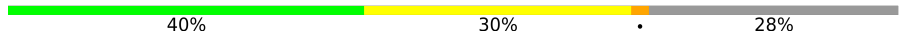
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Mol	Chain	Length	Quality of chain
41	XJ	105	68% 24% 9%
42	QK	129	72% 16% 12%
42	XK	129	71% 15% 12%
43	QL	132	77% 16% 8%
43	XL	132	70% 20% 8%
44	QM	126	70% 21% 8%
44	XM	126	62% 27% 10%
45	QN	61	77% 20%
45	XN	61	77% 20%
46	QO	89	78% 20%
46	XO	89	79% 19%
47	QP	88	67% 23% 7%
47	XP	88	63% 27% 7%
48	QQ	105	84% 10% 6%
48	XQ	105	83% 11% 6%
49	QR	88	64% 13% 23%
49	XR	88	64% 13% 23%
50	QS	93	67% 18% 11%
50	XS	93	72% 17% 11%
51	QT	106	68% 21% 9%
51	XT	106	74% 17% 8%
52	QU	27	70% 15% 15%
52	XU	27	74% 11% 15%
53	QV	77	62% 32% 5%
53	XV	77	64% 26% 9%

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Mol	Chain	Length	Quality of chain
54	QX	25	
54	XX	25	
55	QY	360	
55	XY	360	

## 2 Entry composition [i](#)

There are 58 unique types of molecules in this entry. The entry contains 294929 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	RA	2867	61758	27491	11552	19850	2865	0	0	0
1	YA	2867	61758	27491	11552	19850	2865	0	0	0

- Molecule 2 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	RB	120	2572	1145	476	832	119	0	0	0
2	YB	120	2573	1146	476	832	119	0	0	0

- Molecule 3 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	RD	275	2131	1346	422	360	3	0	0	0
3	YD	275	2136	1349	423	361	3	0	0	0

- Molecule 4 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	RE	204	1559	985	298	270	6	0	0	0
4	YE	204	1559	985	298	270	6	0	0	0

- Molecule 5 is a protein called 50S ribosomal protein L4.



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	RF	203	Total 1584	C 1009	N 298	O 275	S 2	0	0	1
5	YF	203	Total 1580	C 1007	N 297	O 274	S 2	0	0	1

- Molecule 6 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	RG	181	Total 1426	C 916	N 253	O 253	S 4	0	0	0
6	YG	181	Total 1424	C 912	N 259	O 249	S 4	0	0	0

- Molecule 7 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
7	RH	174	Total 1330	C 845	N 248	O 236	S 1	0	0	0
7	YH	173	Total 1324	C 842	N 247	O 234	S 1	0	0	0

- Molecule 8 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
8	RI	147	Total 1094	C 699	N 191	O 203	S 1	0	0	0
8	YI	146	Total 1076	C 687	N 186	O 202	S 1	0	0	0

- Molecule 9 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
9	RN	140	Total 1121	C 722	N 208	O 187	S 4	0	0	0
9	YN	140	Total 1117	C 719	N 207	O 187	S 4	0	0	0

- Molecule 10 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
10	RO	122	Total 933	C 588	N 171	O 170	S 4	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
10	YO	122	933	588	171	170	4	0	0	0

- Molecule 11 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
11	RP	149	1135	706	230	196	3	0	0	0
11	YP	149	1135	706	230	196	3	0	0	0

- Molecule 12 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
12	RQ	141	1122	715	212	188	7	0	0	0
12	YQ	141	1122	715	212	188	7	0	0	0

- Molecule 13 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
13	RR	118	968	604	203	160	1	0	0	0
13	YR	118	968	604	203	160	1	0	0	0

- Molecule 14 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
14	RS	110	877	553	175	149	0	0	0
14	YS	110	870	549	173	148	0	0	0

- Molecule 15 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
15	RT	131	1091	680	225	185	1	0	0	0
15	YT	131	1083	675	224	183	1	0	0	0

- Molecule 16 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
16	RU	116	Total 959	C 608	N 201	O 149	S 1	0	0	0
16	YU	116	Total 959	C 608	N 201	O 149	S 1	0	0	0

- Molecule 17 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
17	RV	101	Total 775	C 498	N 141	O 135	S 1	0	0	0
17	YV	101	Total 771	C 495	N 140	O 135	S 1	0	0	0

- Molecule 18 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
18	RW	112	Total 886	C 557	N 174	O 153	S 2	0	0	0
18	YW	112	Total 886	C 557	N 174	O 153	S 2	0	0	0

- Molecule 19 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
19	RX	95	Total 750	C 488	N 135	O 126	S 1	0	0	0
19	YX	95	Total 750	C 488	N 135	O 126	S 1	0	0	0

- Molecule 20 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
20	RY	107	Total 810	C 520	N 153	O 131	S 6	0	0	0
20	YY	107	Total 810	C 519	N 153	O 132	S 6	0	0	0

- Molecule 21 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
21	RZ	203	Total 1587	C 1011	N 282	O 292	S 2	0	0	0
21	YZ	201	Total 1557	C 995	N 274	O 286	S 2	0	0	0

- Molecule 22 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
22	R0	77	Total 608	C 375	N 129	O 103	S 1	0	0	0
22	Y0	77	Total 608	C 375	N 129	O 103	S 1	0	0	0

- Molecule 23 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
23	R1	97	Total 754	C 475	N 148	O 130	S 1	0	0	0
23	Y1	97	Total 759	C 478	N 149	O 131	S 1	0	0	0

- Molecule 24 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
24	R2	70	Total 588	C 365	N 118	O 103	S 2	0	0	0
24	Y2	70	Total 592	C 368	N 119	O 103	S 2	0	0	0

- Molecule 25 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
25	R3	59	Total 469	C 298	N 90	O 81	0	0	0
25	Y3	59	Total 464	C 296	N 90	O 78	0	0	0

- Molecule 26 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
26	R4	69	Total 546	C 346	N 96	O 99	S 5	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	Y4	69	Total	C	N	O	S	0	0	0
			536	342	98	91	5			

- Molecule 27 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	R5	59	Total	C	N	O	S	0	0	0
			459	288	90	76	5			
27	Y5	59	Total	C	N	O	S	0	0	0
			455	285	89	76	5			

- Molecule 28 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	R6	53	Total	C	N	O	S	0	0	0
			453	281	91	77	4			
28	Y6	53	Total	C	N	O	S	0	0	0
			449	279	91	75	4			

- Molecule 29 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	R7	48	Total	C	N	O	S	0	0	0
			418	257	104	55	2			
29	Y7	48	Total	C	N	O	S	0	0	0
			418	257	104	55	2			

- Molecule 30 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	R8	64	Total	C	N	O	S	0	0	0
			517	331	102	82	2			
30	Y8	64	Total	C	N	O	S	0	0	0
			517	331	102	82	2			

- Molecule 31 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	R9	37	Total	C	N	O	S	0	0	0
			307	188	68	47	4			
31	Y9	37	Total	C	N	O	S	0	0	0
			307	188	68	47	4			

- Molecule 32 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	QA	1500	Total	C	N	O	P	0	0	0
			32246	14358	5975	10413	1500			
32	XA	1504	Total	C	N	O	P	0	0	0
			32331	14396	5990	10441	1504			

- Molecule 33 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	QB	231	Total	C	N	O	S	0	0	0
			1842	1175	330	332	5			
33	XB	231	Total	C	N	O	S	0	0	0
			1825	1167	326	327	5			

- Molecule 34 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	QC	206	Total	C	N	O	S	0	0	0
			1558	979	305	273	1			
34	XC	206	Total	C	N	O	S	0	0	0
			1542	968	300	273	1			

- Molecule 35 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	QD	208	Total	C	N	O	S	0	0	0
			1665	1043	329	286	7			
35	XD	208	Total	C	N	O	S	0	0	0
			1668	1047	330	284	7			

- Molecule 36 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	QE	148	Total	C	N	O	S	0	0	0
			1133	716	214	199	4			
36	XE	148	Total	C	N	O	S	0	0	0
			1133	716	214	199	4			

- Molecule 37 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	QF	100	Total	C	N	O	S	0	0	0
			814	516	144	151	3			
37	XF	100	Total	C	N	O	S	0	0	0
			816	516	146	151	3			

- Molecule 38 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	QG	155	Total	C	N	O	S	0	0	0
			1235	769	244	216	6			
38	XG	155	Total	C	N	O	S	0	0	0
			1229	766	241	216	6			

- Molecule 39 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	QH	137	Total	C	N	O	S	0	0	0
			1098	694	210	192	2			
39	XH	137	Total	C	N	O	S	0	0	0
			1088	689	206	191	2			

- Molecule 40 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
40	QI	127	Total	C	N	O	0	0	0
			986	625	193	168			
40	XI	126	Total	C	N	O	0	0	0
			966	613	186	167			

- Molecule 41 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
41	QJ	97	Total	C	N	O	0	0	0
			719	446	142	131			
41	XJ	96	Total	C	N	O	0	0	0
			710	442	137	131			

- Molecule 42 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	QK	114	Total	C	N	O	S	0	0	0
			834	520	156	155	3			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
42	XK	114	833	519	156	155	3	0	0	0

- Molecule 43 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
43	QL	122	932	586	185	159	2	0	0	0
43	XL	122	932	586	185	159	2	0	0	0

- Molecule 44 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
44	QM	116	914	564	189	159	2	0	0	0
44	XM	114	895	550	186	157	2	0	0	0

- Molecule 45 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
45	QN	60	492	312	104	72	4	0	0	0
45	XN	60	492	312	104	72	4	0	0	0

- Molecule 46 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
46	QO	88	728	456	144	126	2	0	0	0
46	XO	88	728	456	144	126	2	0	0	0

- Molecule 47 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
47	QP	82	681	433	134	113	1	0	0	0
47	XP	82	677	430	133	113	1	0	0	0



- Molecule 48 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
48	QQ	99	Total 823	C 528	N 151	O 142	S 2	0	0	0
48	XQ	99	Total 823	C 528	N 151	O 142	S 2	0	0	0

- Molecule 49 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
49	QR	68	Total 555	C 355	N 108	O 92	S	0	0	0
49	XR	68	Total 555	C 355	N 108	O 92	S	0	0	0

- Molecule 50 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
50	QS	83	Total 648	C 415	N 120	O 111	S 2	0	0	0
50	XS	83	Total 645	C 410	N 118	O 115	S 2	0	0	0

- Molecule 51 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
51	QT	96	Total 732	C 449	N 157	O 124	S 2	0	0	0
51	XT	98	Total 733	C 451	N 154	O 126	S 2	0	0	0

- Molecule 52 is a protein called 30S ribosomal protein Thx.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
52	QU	23	Total 199	C 122	N 48	O 29	0	0	0
52	XU	23	Total 199	C 122	N 48	O 29	0	0	0

- Molecule 53 is a RNA chain called P-site tRNA fMet.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
53	QV	77	Total 1640	C 732	N 297	O 535	P 76	0	0	0
53	XV	77	Total 1644	C 732	N 297	O 538	P 77	0	0	0

- Molecule 54 is a RNA chain called messenger RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
54	QX	9	Total 193	C 87	N 37	O 60	P 9	0	0	0
54	XX	10	Total 215	C 97	N 42	O 66	P 10	0	0	0

- Molecule 55 is a protein called Peptide chain release factor 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
55	QY	259	Total 2014	C 1235	N 382	O 389	S 8	0	0	0
55	XY	260	Total 2022	C 1241	N 383	O 390	S 8	0	0	0

- Molecule 56 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	RA	1032	Total 1032	Mg 1032	0	0
56	RB	22	Total 22	Mg 22	0	0
56	RD	15	Total 15	Mg 15	0	0
56	RE	7	Total 7	Mg 7	0	0
56	RF	11	Total 11	Mg 11	0	0
56	RG	4	Total 4	Mg 4	0	0
56	RN	2	Total 2	Mg 2	0	0
56	RO	1	Total 1	Mg 1	0	0
56	RP	2	Total 2	Mg 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	RQ	5	Total Mg 5 5	0	0
56	RR	4	Total Mg 4 4	0	0
56	RS	1	Total Mg 1 1	0	0
56	RT	3	Total Mg 3 3	0	0
56	RU	3	Total Mg 3 3	0	0
56	RV	3	Total Mg 3 3	0	0
56	RW	2	Total Mg 2 2	0	0
56	RX	1	Total Mg 1 1	0	0
56	RY	1	Total Mg 1 1	0	0
56	R0	7	Total Mg 7 7	0	0
56	R1	5	Total Mg 5 5	0	0
56	R3	2	Total Mg 2 2	0	0
56	R5	1	Total Mg 1 1	0	0
56	R7	3	Total Mg 3 3	0	0
56	R9	1	Total Mg 1 1	0	0
56	QA	262	Total Mg 262 262	0	0
56	QB	1	Total Mg 1 1	0	0
56	QD	2	Total Mg 2 2	0	0
56	QE	2	Total Mg 2 2	0	0
56	QF	1	Total Mg 1 1	0	0
56	QG	3	Total Mg 3 3	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	QH	1	Total Mg 1 1	0	0
56	QI	1	Total Mg 1 1	0	0
56	QJ	1	Total Mg 1 1	0	0
56	QL	2	Total Mg 2 2	0	0
56	QN	1	Total Mg 1 1	0	0
56	QO	1	Total Mg 1 1	0	0
56	QQ	1	Total Mg 1 1	0	0
56	QR	1	Total Mg 1 1	0	0
56	QT	1	Total Mg 1 1	0	0
56	QV	6	Total Mg 6 6	0	0
56	YA	749	Total Mg 749 749	0	0
56	YB	20	Total Mg 20 20	0	0
56	YD	9	Total Mg 9 9	0	0
56	YE	6	Total Mg 6 6	0	0
56	YF	2	Total Mg 2 2	0	0
56	YG	2	Total Mg 2 2	0	0
56	YI	1	Total Mg 1 1	0	0
56	YN	1	Total Mg 1 1	0	0
56	YO	1	Total Mg 1 1	0	0
56	YP	1	Total Mg 1 1	0	0
56	YQ	3	Total Mg 3 3	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	YR	1	Total Mg 1 1	0	0
56	YT	3	Total Mg 3 3	0	0
56	YV	1	Total Mg 1 1	0	0
56	YW	2	Total Mg 2 2	0	0
56	YX	1	Total Mg 1 1	0	0
56	Y0	1	Total Mg 1 1	0	0
56	Y1	1	Total Mg 1 1	0	0
56	Y5	2	Total Mg 2 2	0	0
56	Y7	1	Total Mg 1 1	0	0
56	Y8	2	Total Mg 2 2	0	0
56	XA	187	Total Mg 187 187	0	0
56	XE	2	Total Mg 2 2	0	0
56	XF	4	Total Mg 4 4	0	0
56	XJ	1	Total Mg 1 1	0	0
56	XL	1	Total Mg 1 1	0	0
56	XT	1	Total Mg 1 1	0	0
56	XV	4	Total Mg 4 4	0	0
56	XY	1	Total Mg 1 1	0	0

- Molecule 57 is ZINC ION (three-letter code: ZN) (formula: Zn).

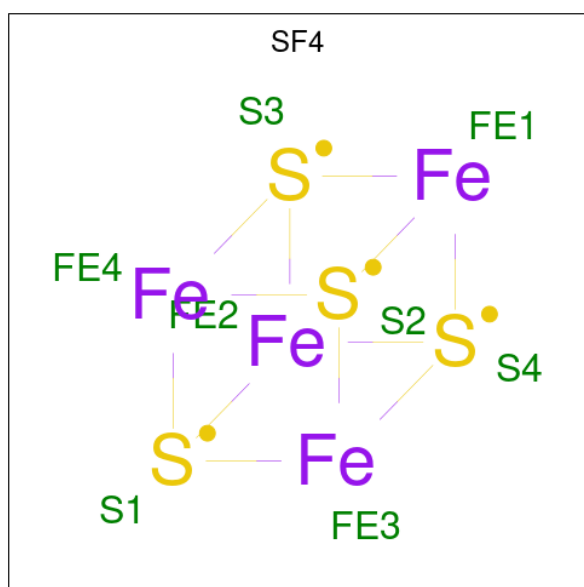
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	RY	1	Total Zn 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	R4	1	Total Zn 1 1	0	0
57	R5	1	Total Zn 1 1	0	0
57	R6	1	Total Zn 1 1	0	0
57	R9	1	Total Zn 1 1	0	0
57	QN	1	Total Zn 1 1	0	0
57	YY	1	Total Zn 1 1	0	0
57	Y4	1	Total Zn 1 1	0	0
57	Y5	1	Total Zn 1 1	0	0
57	Y6	1	Total Zn 1 1	0	0
57	Y9	1	Total Zn 1 1	0	0
57	XN	1	Total Zn 1 1	0	0

- Molecule 58 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).

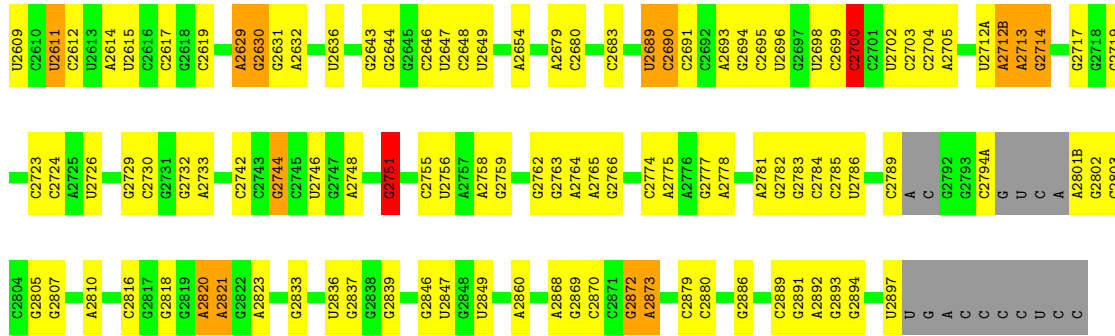


<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>			<b>ZeroOcc</b>	<b>AltConf</b>
58	QD	1	Total 8	Fe 4	S 4	0	0
58	XD	1	Total 8	Fe 4	S 4	0	0

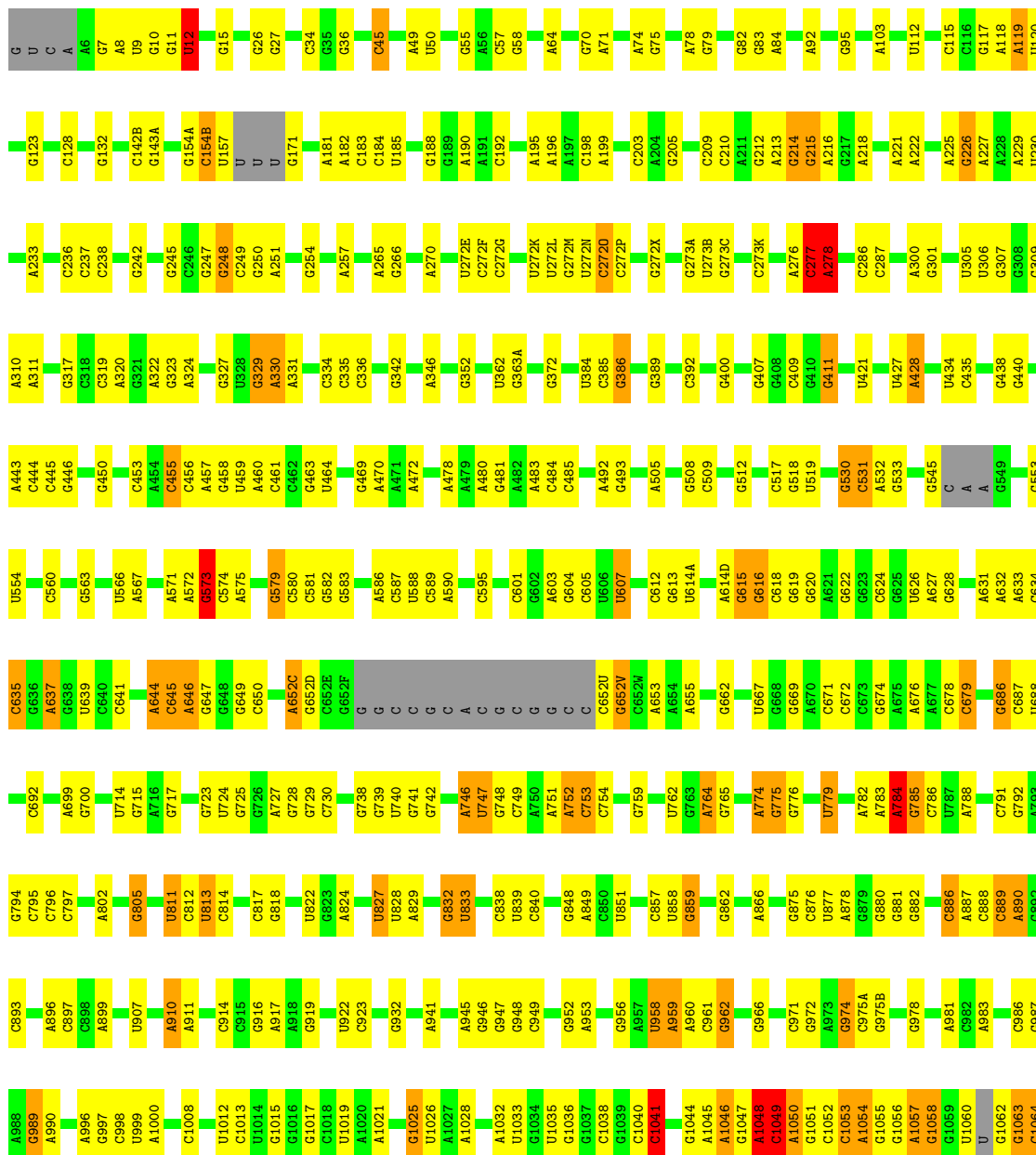




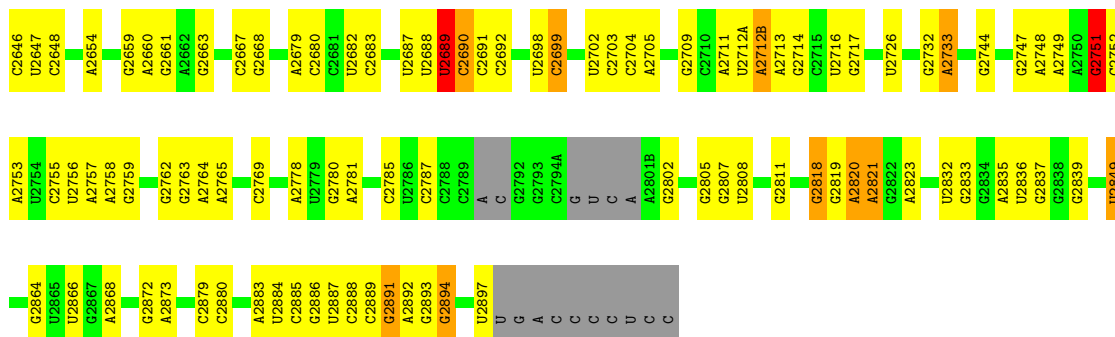




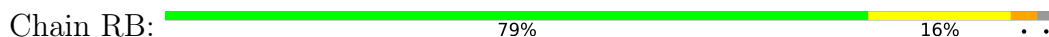
• Molecule 1: 23S rRNA



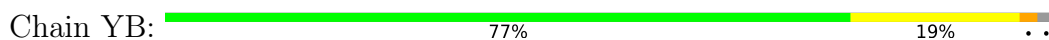
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C1135	G1136	U1141	U1142A	U1142B	A1143	G1151	C1152	C1153	G1154	A1155	A1156	G1157	G1164	U1165	U1166	C1166	A1167	G1171	G	A	U	C	A	U	U	C	A	U1178	G1184	U1188	A1189	G1190	U1211	G1212	C1218	G1219	A1220	G1236	G1239	U1240	G1250	A1253	G1256	G1260	C1261	G1266	U1267	A1268	C1386	A1496					
C1270	G1271	U1272	U1273	A1278	G1283	A1284	G1285	A1286	A1287	U1292	C1293	G1296	U1300	A1301	A1302	G1303	A1308	G1309	U1312	C1313	C1314	C1315	U1316	A1317	C1318	A1328	U1341	U1352	U1357	G1358	A1359	G1364	A1365	G1368	G1369	U1372	A1378	A1379	G1380	A1384	G1385	C1386	A1496												
U1396	U1397	C1404	U1405	U1406	C1407	C1408	A1411	G1412	G1416	C1417	G1418	A1419	U1420	G1421	G1422	G1423	A1427	C1428	G1429	C1430	U1431	C1432	U1433	A1445A	G1450A	C1450B	C1451	G1455	G1459	C1467	G1470	A1471	A1472	G1473	G1478	G1479	G1482	A1486	G1487	A1490	G1491	C1492	C1493	A1496											
U1497	G1500	A1507	C1508	C1509A	A1509B	U1514	G1515	G1520	G1525	U1526	C1530	U1531	C1532	G1533	U	A	C1536	G1539	A1542	C1543	C1547	A1554	C1557	A1558	G1559	A1566	A1569	A1570	A1571	C1577	U1578	A1580	G1581	C1582	A1583	C1584	A1586	A1587	C1588	G1593	G1594	G1595	A1701												
C1598	C1599	U1602	A1608	A1609	A1610	C1611	C1617	A1618	C1625	C1636	A1637	C1638	U1639	C1640	A1641	G1642	G1645	C1646	G1647	C1648	G1649	G1650	G1651	A1654	C1657	C1658	A1664	A1668	A1669	C1670	U1671	C1672	U1673	G1674	C1675	C1683	C1684	U1688	U1693	A1696	A1697	A1698	G1699	A1700	A1701										
G1702	G1703	U1709	C1710	A1719	U1720	U1721	U1722	U1739	G1740	A1741	G1756	U1762	G1763	G1764	G1769	A1773	G1776	A1780	C1781	C1782	A1786	A1791	U1794	C1795	U1796	C1797	U1798	G1799	C1800	G1801	A1802	A1803	C1806	G1807	G1811	A1812	G1813	G1814	G1815	G1816	G1817	U1820	G1823												
G1826	A1829	U1834	G1835	A1847	A1848	A1854	C1866	A1876	A1877	G1878	A1889	A1890	G1899	A1900	G1906	U1911	A1912	A1913	A1914	U1915	A1916	U1917	C1920	G1929	G1930	U1931	A1932	G1933	C1934	G1935	A1936	A1937	A1938	U1939	C1942	U1955	C1962	G1963	C2003	G1964	C1965	A1966	C1967	A1970	A1971										
A1972	U1991	G1992	U1993	G1997	A2001	G2002	G2003	G2004	G2012	A2013	A2014	A2018	A2019	A2020	G2023	U2028	G2029	A2031	A2032	A2033	U2034	G2035	C2036	C2043	U2047	C2055	G2056	A2060	G2061	A2062	C2063	C2064	C2065	C2066	U2067	G2069	G2070	A2071	G2072	C2073	U2074	U2075	U2076	A2077	C2078	U2079									
G2080	C2081	A2082	G2083	U2086	G2087	U2096	U2099	C2103	G2104	C2105	G2106	C2107	C2108	U2109	C2110	G2111	U2112	U2113	G2114	G2115	G2116	A2117	C2118	A2119	G2120	G2121	U2122	G2123	A2126	G2127	C2128	C2129	U2130	U2132	G2133	A2134	A2135	C2136	C2137	C2138	C2139	C2140	G2141	C2142	C2143	C2144	G2145	C2146	G2147	U2150	G2151	G2152			
G2153	G2154	G2155	G2156	G2157	A2158	C2159	C2160	C2161	G2162	G2165	G2166	G2167	G2168	A2171	U2172	A2173	A2176	U2180	G2181	G2182	C2183	C2184	C2185	G2186	G2187	G2188	U2189	G2190	G2191	A2192	G2193	C2194	A2198	C2201	G2206	G2207	A2208	U2218	A2225	C2226	U2233	G2234	G2237	G2238	G2239	G2242	U2243	U2244							
A2247	C2248	U2249	G2250	G2251	G2252	G2253	C2261	U2262	C2263	C2264	U2265	A2266	A2267	A2268	A2269	U2272	A2273	A2274	C2275	G2276	G2277	A2278	G2279	G2280	C2283	C2284	C2285	A2286	A2287	A2288	G2289	G2293	G2294	U2296	C2297	A2298	G2304	A2305	C2306	G2307	G2308	U2312	C2313	C2314	G2315	C2316	G2317	G2318	G2319	A2320	A2321	A2322	G2325		
C2326	A2327	A2328	G2329	G2330	G2331	G2334	A2335	A2336	C2342	C2343	U2344	G2345	A2346	C2347	C2350	C2355	G2358	C2359	A2360	A2361	C2364	G2372	G2373	C2374	C2381	G2382	G2383	G2384	C2385	C2386	A2387	A2388	G2389	U2390	C2391	G2400	G2405	U2406	G2410	G2413	G2414	G2415	G2416	A2422	A2425	G2429									
A2430	U2431	A2435	U2438	A2439	C2440	C2441	G2447	A2448	G2455	C2456	A2456	U2461	U2462	C2463	C2467	C2473	A2474	A2475	A2476	C2477	A2478	G2486	G2487	U2493	G2494	G2495	C2496	A2497	C2498	C2501	G2502	U2503	U2504	G2505	U2506	G2509	G2516	C2517	U2518	C2519	G2520	G2521	C2522	G2523	G2524	G2525	G2526								
G2529	A2530	G2549	U2552	G2553	U2554	G2557	A2561	A2564	A2565	U2566	G2567	U2568	G2569	G2570	C2571	A2572	C2573	G2574	G2578	G2582	G2583	G2586	C2591	U2592	U2593	C2594	A2602	U2605	G2608	U2609	C2610	U2611	C2612	G2619	G2627	C2628	G2629	G2630	G2631	U2636	G2641														



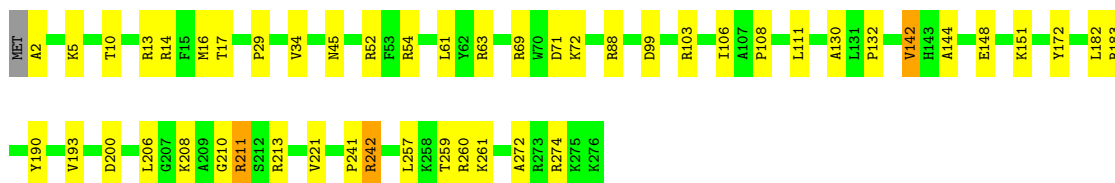
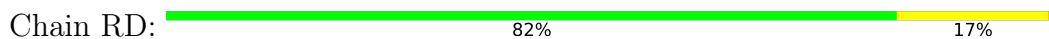
• Molecule 2: 5S rRNA



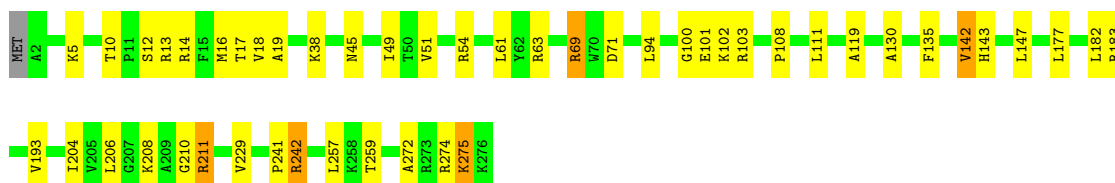
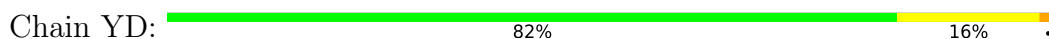
• Molecule 2: 5S rRNA



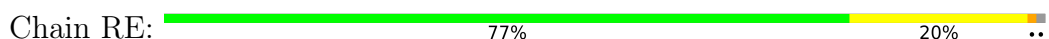
• Molecule 3: 50S ribosomal protein L2

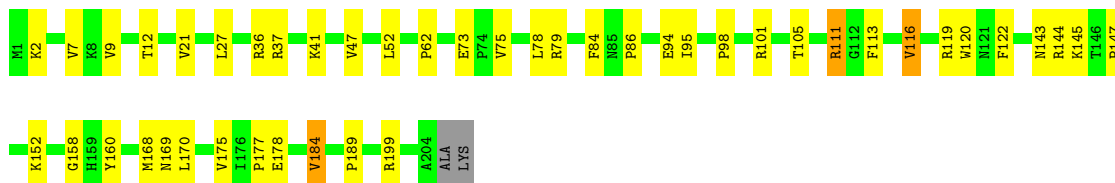


• Molecule 3: 50S ribosomal protein L2

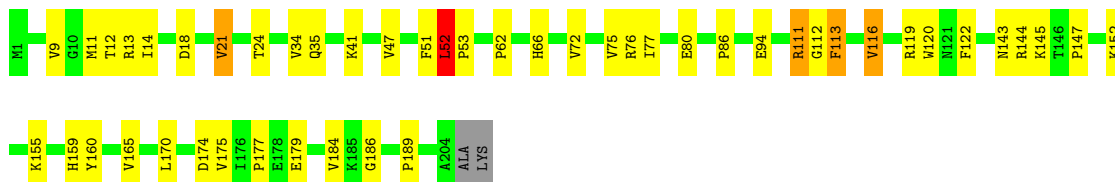
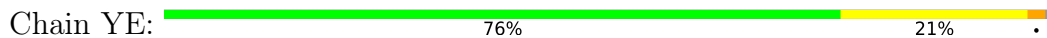


• Molecule 4: 50S ribosomal protein L3

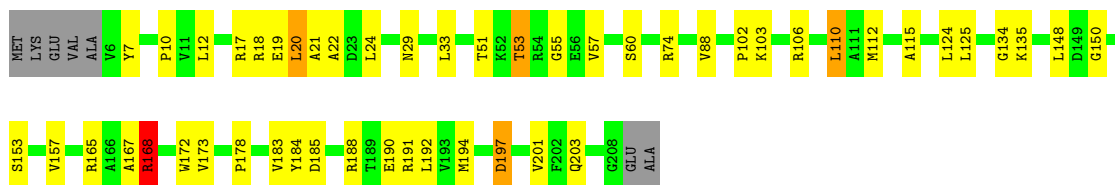




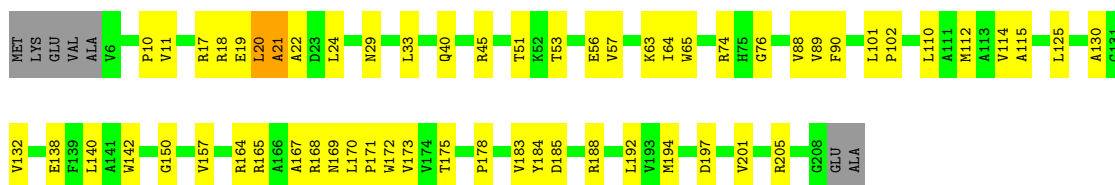
- Molecule 4: 50S ribosomal protein L3



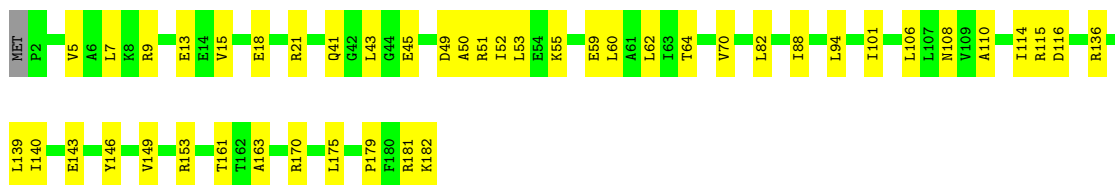
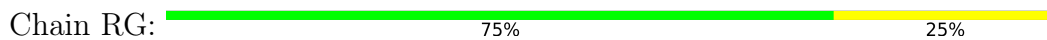
- Molecule 5: 50S ribosomal protein L4



- Molecule 5: 50S ribosomal protein L4



- Molecule 6: 50S ribosomal protein L5

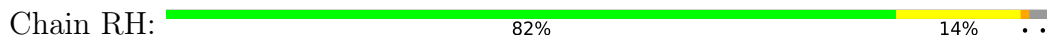


- Molecule 6: 50S ribosomal protein L5





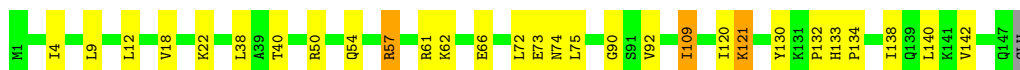
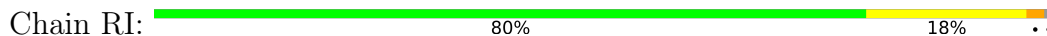
- Molecule 7: 50S ribosomal protein L6



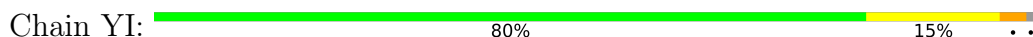
- Molecule 7: 50S ribosomal protein L6



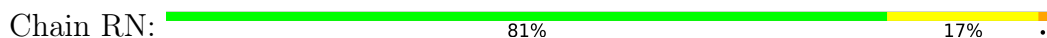
- Molecule 8: 50S ribosomal protein L9



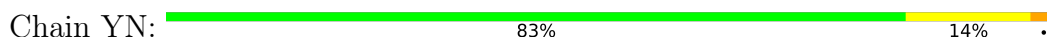
- Molecule 8: 50S ribosomal protein L9

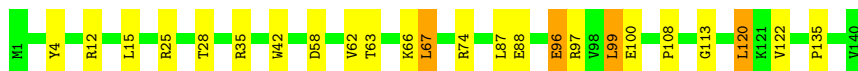


- Molecule 9: 50S ribosomal protein L13

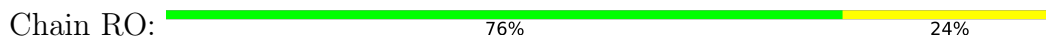


- Molecule 9: 50S ribosomal protein L13

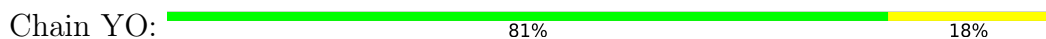




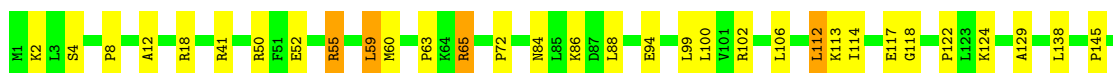
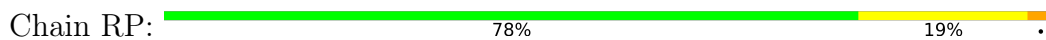
- Molecule 10: 50S ribosomal protein L14



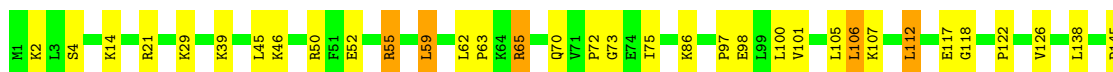
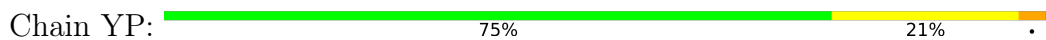
- Molecule 10: 50S ribosomal protein L14



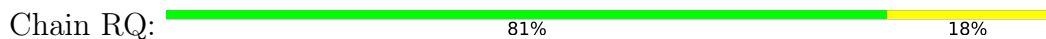
- Molecule 11: 50S ribosomal protein L15



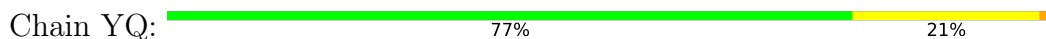
- Molecule 11: 50S ribosomal protein L15



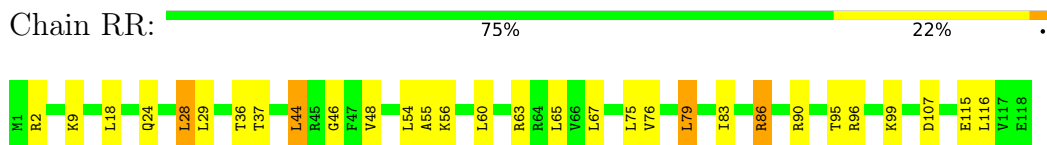
- Molecule 12: 50S ribosomal protein L16



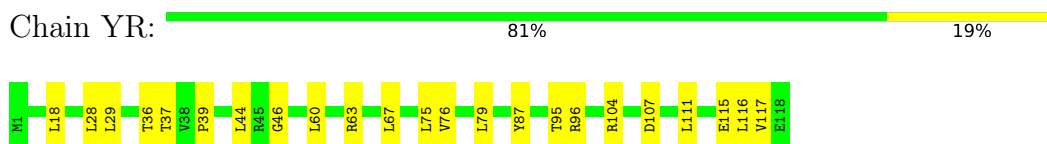
- Molecule 12: 50S ribosomal protein L16



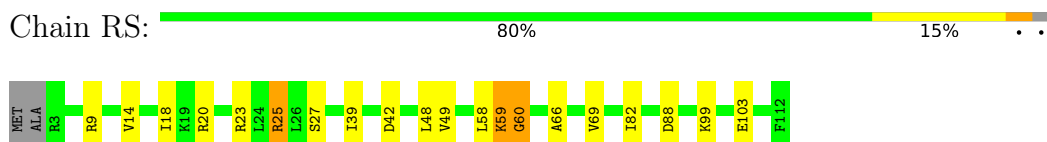
- Molecule 13: 50S ribosomal protein L17



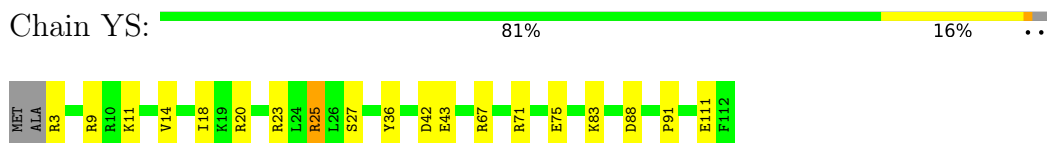
- Molecule 13: 50S ribosomal protein L17



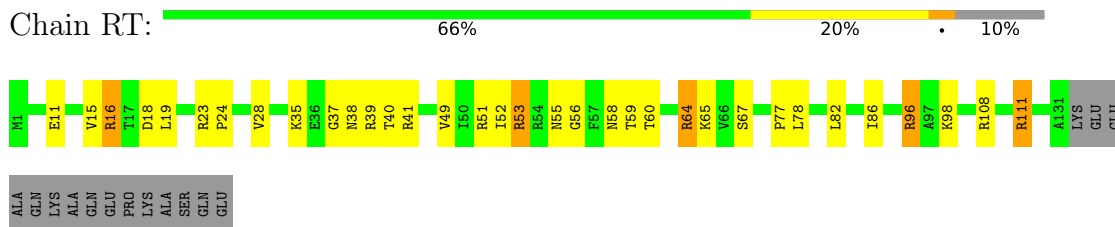
- Molecule 14: 50S ribosomal protein L18



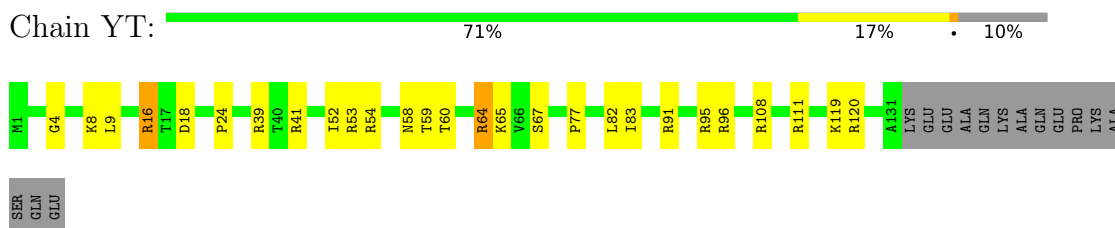
- Molecule 14: 50S ribosomal protein L18



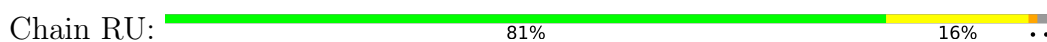
- Molecule 15: 50S ribosomal protein L19



- Molecule 15: 50S ribosomal protein L19



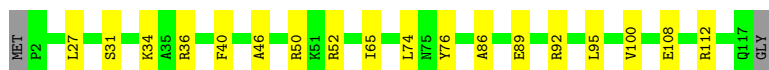
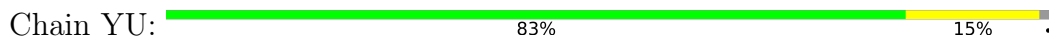
- Molecule 16: 50S ribosomal protein L20



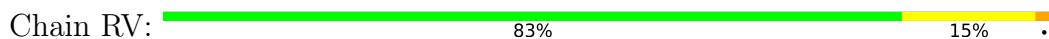




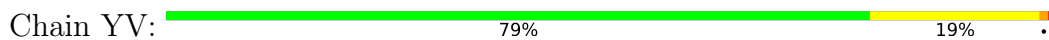
- Molecule 16: 50S ribosomal protein L20



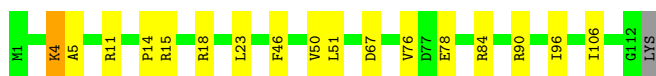
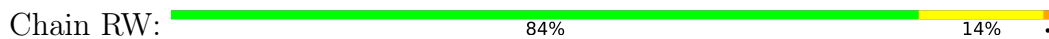
- Molecule 17: 50S ribosomal protein L21



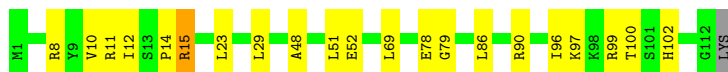
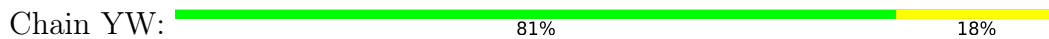
- Molecule 17: 50S ribosomal protein L21



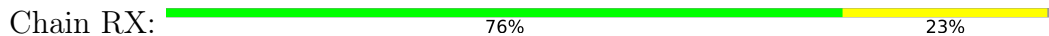
- Molecule 18: 50S ribosomal protein L22



- Molecule 18: 50S ribosomal protein L22



- Molecule 19: 50S ribosomal protein L23

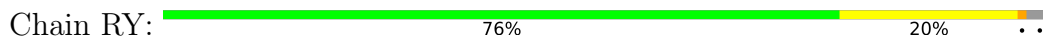


- Molecule 19: 50S ribosomal protein L23

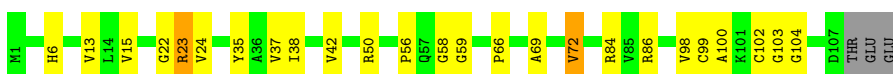
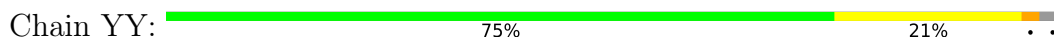




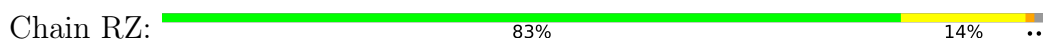
- Molecule 20: 50S ribosomal protein L24



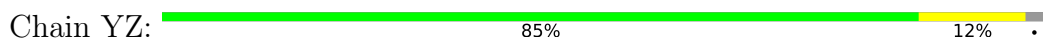
- Molecule 20: 50S ribosomal protein L24



- Molecule 21: 50S ribosomal protein L25



- Molecule 21: 50S ribosomal protein L25



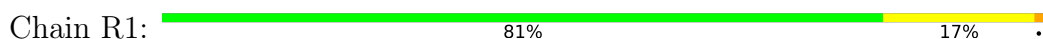
- Molecule 22: 50S ribosomal protein L27



- Molecule 22: 50S ribosomal protein L27



- Molecule 23: 50S ribosomal protein L28





- Molecule 23: 50S ribosomal protein L28

Chain Y1: 76% 21% ..



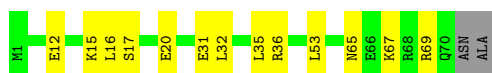
- Molecule 24: 50S ribosomal protein L29

Chain R2: 75% 22% .



- Molecule 24: 50S ribosomal protein L29

Chain Y2: 79% 18% .



- Molecule 25: 50S ribosomal protein L30

Chain R3: 87% 12% ..



- Molecule 25: 50S ribosomal protein L30

Chain Y3: 78% 18% ..



- Molecule 26: 50S ribosomal protein L31

Chain R4: 58% 35% ...



- Molecule 26: 50S ribosomal protein L31

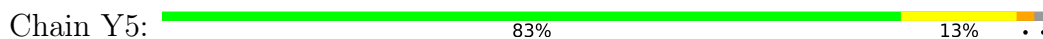
Chain Y4: 63% 30% ...



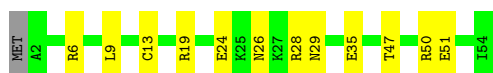
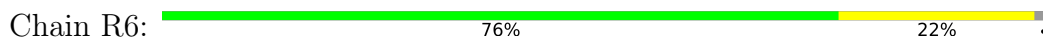
- Molecule 27: 50S ribosomal protein L32



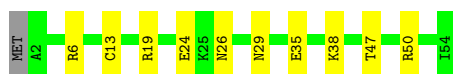
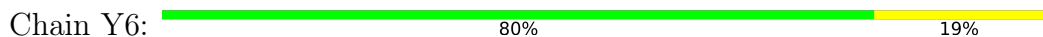
- Molecule 27: 50S ribosomal protein L32



- Molecule 28: 50S ribosomal protein L33



- Molecule 28: 50S ribosomal protein L33



- Molecule 29: 50S ribosomal protein L34



- Molecule 29: 50S ribosomal protein L34



- Molecule 30: 50S ribosomal protein L35





• Molecule 30: 50S ribosomal protein L35



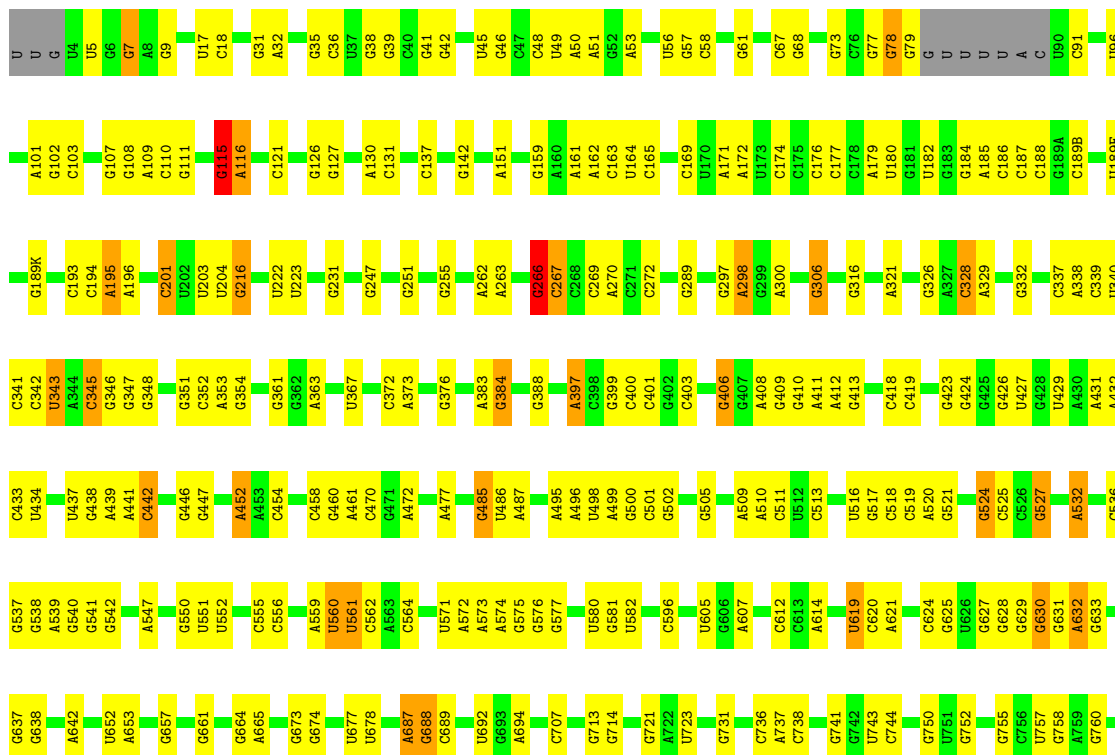
• Molecule 31: 50S ribosomal protein L36

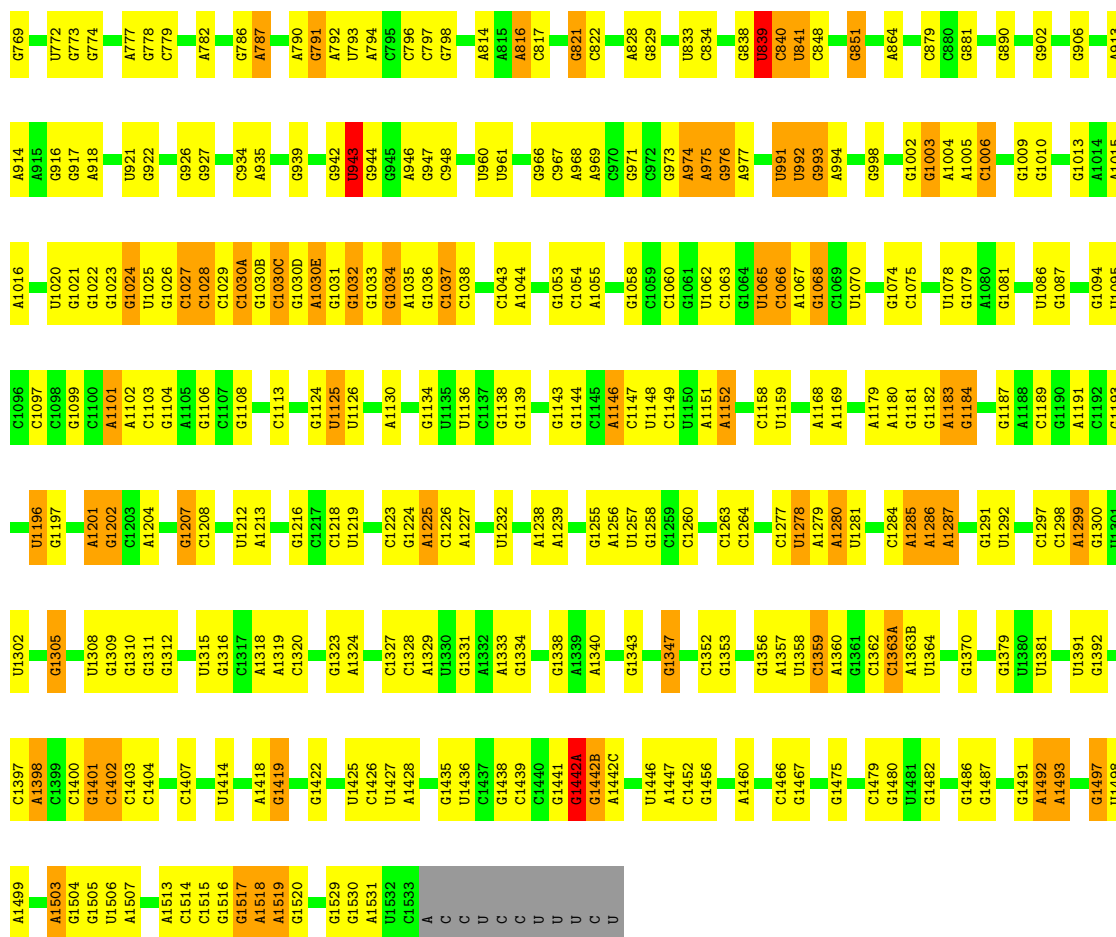


• Molecule 31: 50S ribosomal protein L36



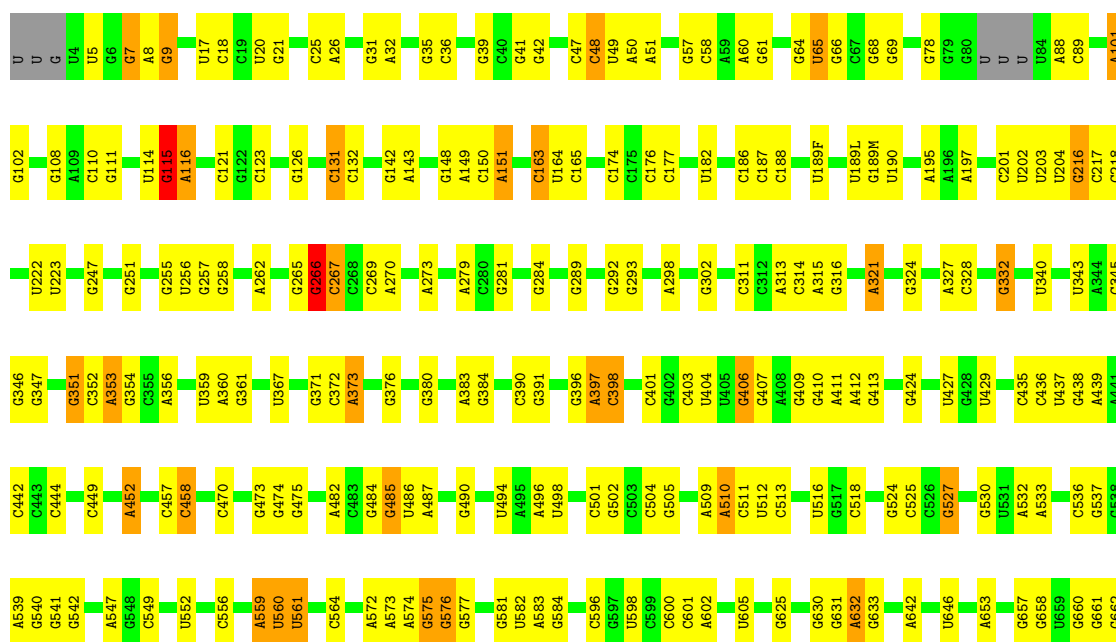
• Molecule 32: 16S rRNA

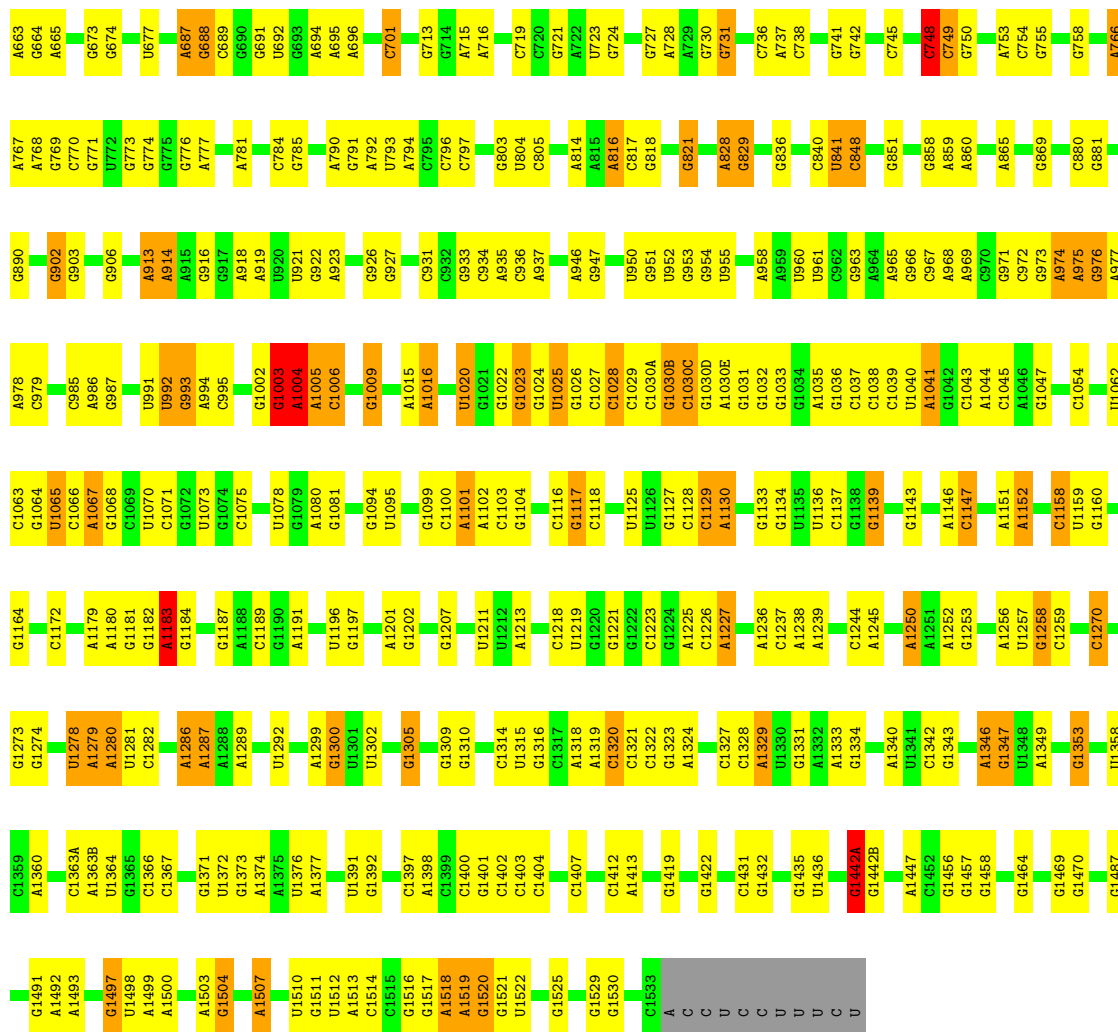




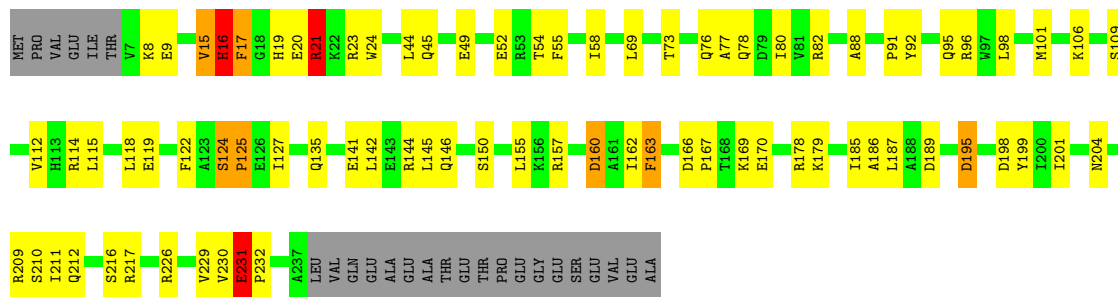
- Molecule 32: 16S rRNA

Chain XA: 60% 32% 6%

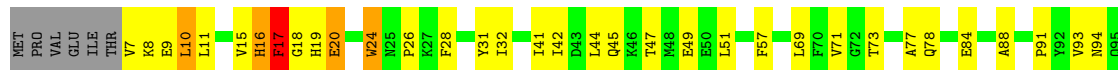


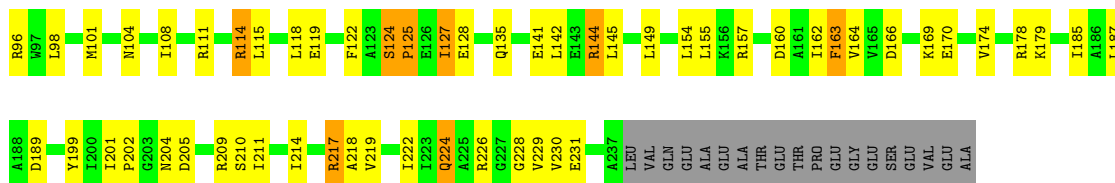


● Molecule 33: 30S ribosomal protein S2

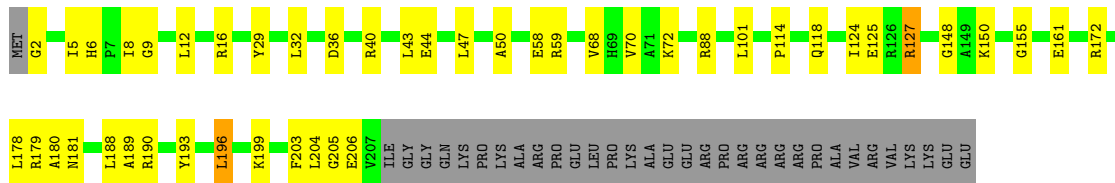


● Molecule 33: 30S ribosomal protein S2

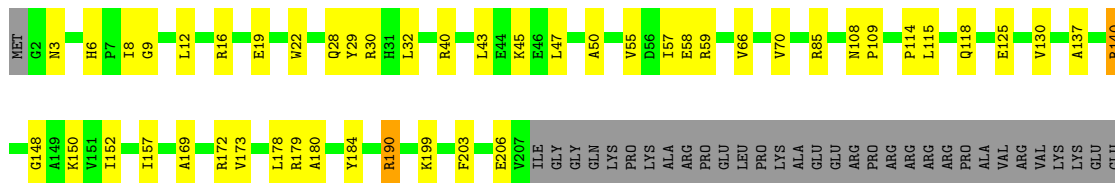




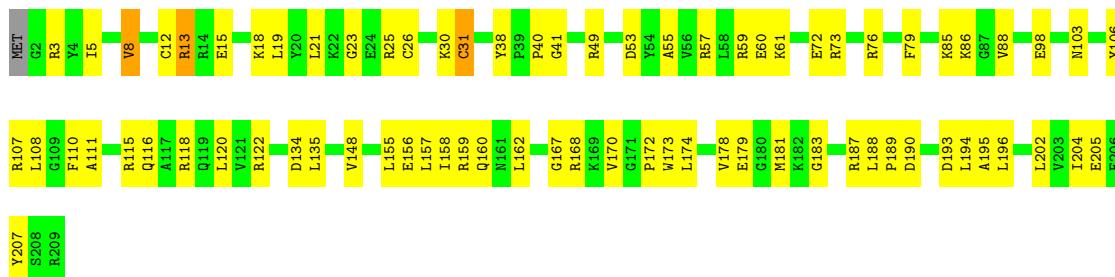
• Molecule 34: 30S ribosomal protein S3



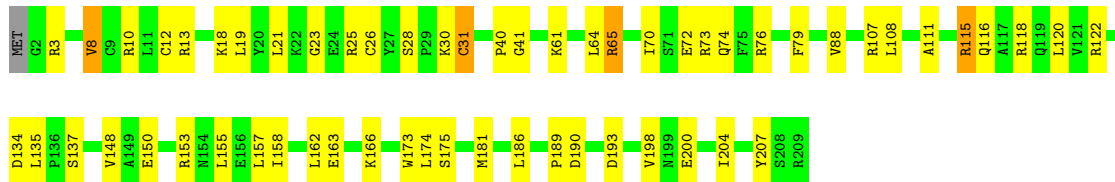
• Molecule 34: 30S ribosomal protein S3



• Molecule 35: 30S ribosomal protein S4



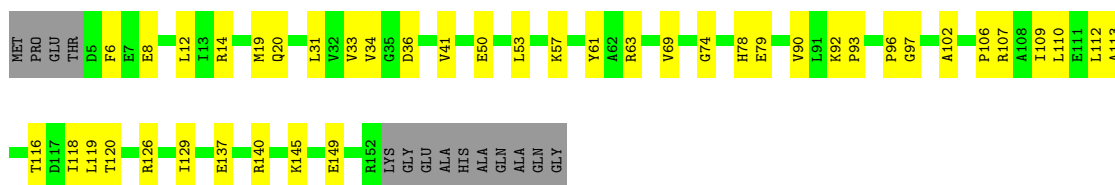
• Molecule 35: 30S ribosomal protein S4





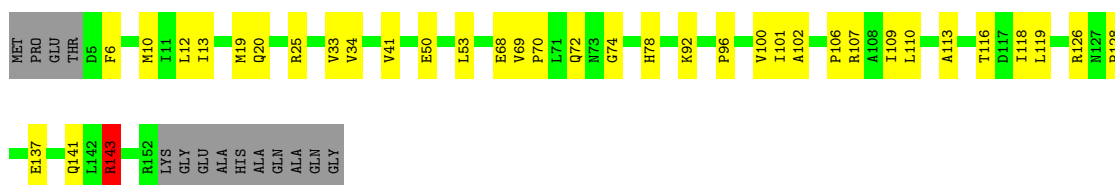
- Molecule 36: 30S ribosomal protein S5

Chain QE:  65% 26% 9%



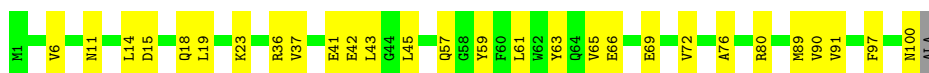
- Molecule 36: 30S ribosomal protein S5

Chain XE:  69% 22% 9%




- Molecule 37: 30S ribosomal protein S6

Chain QF:  71% 28% 1%




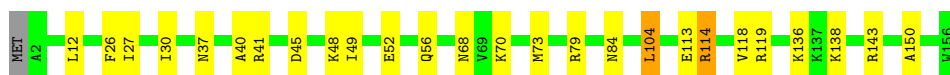
- Molecule 37: 30S ribosomal protein S6

Chain XF:  86% 12% 2%




- Molecule 38: 30S ribosomal protein S7

Chain QG:  83% 15% 2%




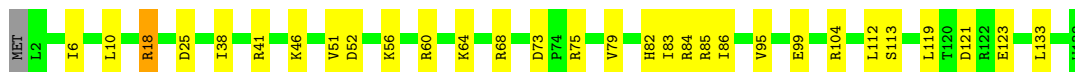
- Molecule 38: 30S ribosomal protein S7

Chain XG:  83% 15% 2%




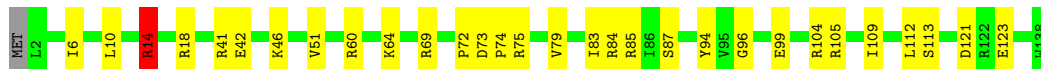
- Molecule 39: 30S ribosomal protein S8

Chain QH:  78% 21% ..



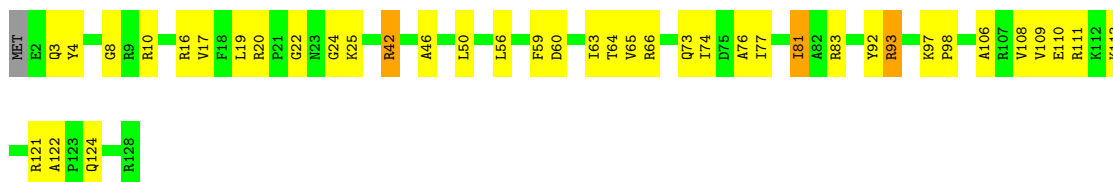
- Molecule 39: 30S ribosomal protein S8

Chain XH:  78% 21% ..



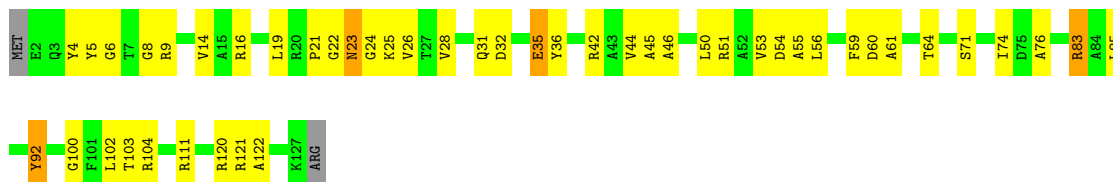
- Molecule 40: 30S ribosomal protein S9

Chain QI:  68% 29% ..



- Molecule 40: 30S ribosomal protein S9

Chain XI:  62% 34% ..



- Molecule 41: 30S ribosomal protein S10

Chain QJ:  57% 33% 8%



- Molecule 41: 30S ribosomal protein S10

Chain XJ:  68% 24% 9%



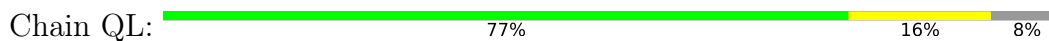
• Molecule 42: 30S ribosomal protein S11



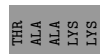
• Molecule 42: 30S ribosomal protein S11



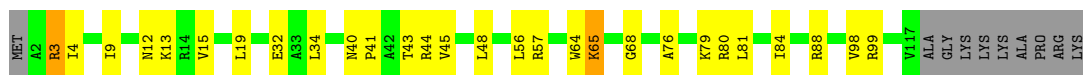
• Molecule 43: 30S ribosomal protein S12



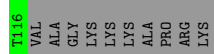
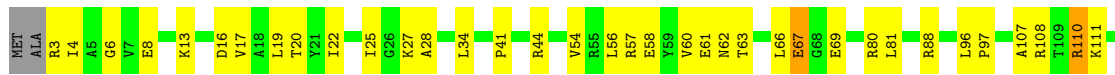
• Molecule 43: 30S ribosomal protein S12




• Molecule 44: 30S ribosomal protein S13



• Molecule 44: 30S ribosomal protein S13




• Molecule 45: 30S ribosomal protein S14 type Z

Chain QN:  77% 20% ..




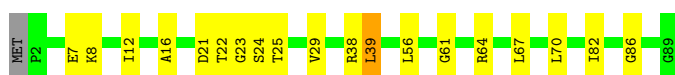
- Molecule 45: 30S ribosomal protein S14 type Z

Chain XN:  77% 20% ..




- Molecule 46: 30S ribosomal protein S15

Chain QO:  78% 20% ..



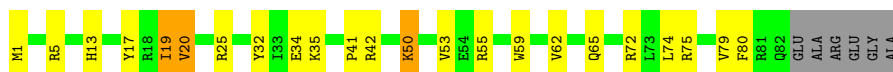
- Molecule 46: 30S ribosomal protein S15

Chain XO:  79% 19% ..



- Molecule 47: 30S ribosomal protein S16

Chain QP:  67% 23% 7% ..




- Molecule 47: 30S ribosomal protein S16

Chain XP:  63% 27% 7% ..




- Molecule 48: 30S ribosomal protein S17

Chain QQ:  84% 10% 6% ..



- Molecule 48: 30S ribosomal protein S17

Chain XQ:  83% 11% 6%



- Molecule 49: 30S ribosomal protein S18

Chain QR:  64% 13% 23%



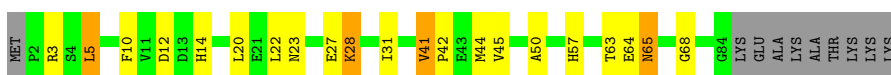
- Molecule 49: 30S ribosomal protein S18

Chain XR:  64% 13% 23%



- Molecule 50: 30S ribosomal protein S19

Chain QS:  67% 18% 11%



- Molecule 50: 30S ribosomal protein S19

Chain XS:  72% 17% 11%




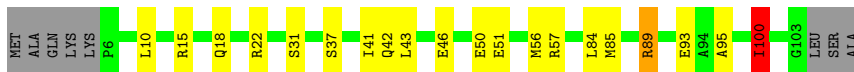
- Molecule 51: 30S ribosomal protein S20

Chain QT:  68% 21% 9%



- Molecule 51: 30S ribosomal protein S20

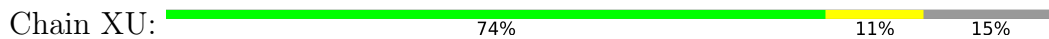
Chain XT:  74% 17% 8%



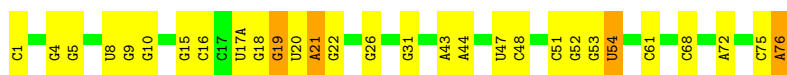
- Molecule 52: 30S ribosomal protein Thx



- Molecule 52: 30S ribosomal protein Thx



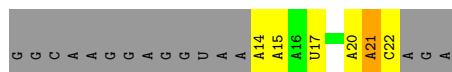
- Molecule 53: P-site tRNA fMet



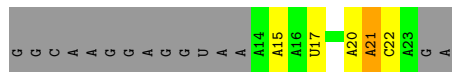
- Molecule 53: P-site tRNA fMet



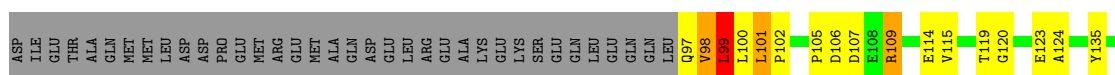
- Molecule 54: messenger RNA



- Molecule 54: messenger RNA

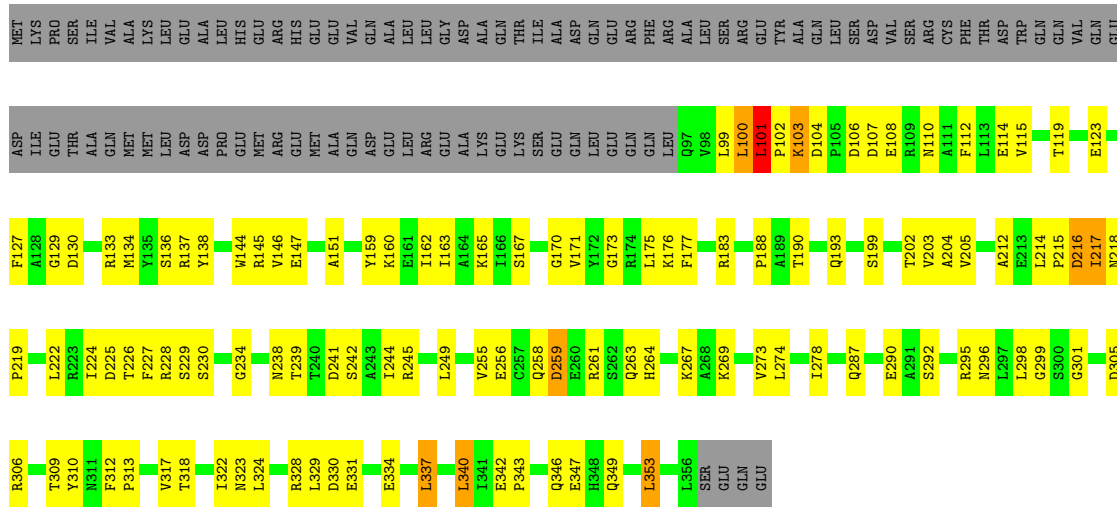


- Molecule 55: Peptide chain release factor 1





• Molecule 55: Peptide chain release factor 1



## 4 Data and refinement statistics

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	209.51Å 450.89Å 622.07Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.86 – 3.04	Depositor
% Data completeness (in resolution range)	99.3 (49.86-3.04)	Depositor
$R_{merge}$	0.35	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.65 (at 3.07Å)	Xtrriage
Refinement program	PHENIX, PHENIX	Depositor
R, $R_{free}$	0.246 , 0.279	Depositor
Wilson B-factor (Å <sup>2</sup> )	65.2	Xtrriage
Anisotropy	0.225	Xtrriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.37$ , $\langle L^2 \rangle = 0.20$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	294929	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	82.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.69% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



## 5 Model quality i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: UR3, 5MU, 2MG, ZN, OMG, MG, PSU, 0TD, 2MA, 2MU, 4OC, 5MC, MA6, M2G, 7MG, SF4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	RA	0.43	0/68901	1.00	55/107544 (0.1%)
1	YA	0.51	1/68901 (0.0%)	1.10	180/107544 (0.2%)
2	RB	0.35	0/2876	0.90	0/4486
2	YB	0.43	0/2878	1.00	1/4490 (0.0%)
3	RD	0.38	0/2181	0.64	1/2940 (0.0%)
3	YD	0.40	0/2186	0.66	1/2944 (0.0%)
4	RE	0.37	0/1592	0.60	0/2149
4	YE	0.38	0/1592	0.65	1/2149 (0.0%)
5	RF	0.36	0/1619	0.61	2/2193 (0.1%)
5	YF	0.42	0/1615	0.61	0/2188
6	RG	0.29	0/1451	0.54	0/1961
6	YG	0.34	0/1449	0.57	0/1957
7	RH	0.31	0/1356	0.54	1/1834 (0.1%)
7	YH	0.35	0/1350	0.57	1/1826 (0.1%)
8	RI	0.29	0/1109	0.57	0/1512
8	YI	0.34	0/1091	0.60	1/1490 (0.1%)
9	RN	0.36	0/1148	0.56	0/1547
9	YN	0.35	0/1144	0.55	0/1543
10	RO	0.34	0/943	0.58	0/1269
10	YO	0.42	1/943 (0.1%)	0.61	0/1269
11	RP	0.35	0/1152	0.60	0/1533
11	YP	0.41	0/1152	0.66	0/1533
12	RQ	0.35	0/1143	0.62	0/1527
12	YQ	0.40	0/1143	0.66	0/1527
13	RR	0.34	0/982	0.62	0/1312
13	YR	0.34	0/982	0.62	0/1312
14	RS	0.35	0/887	0.59	0/1180
14	YS	0.37	0/880	0.62	0/1172
15	RT	0.36	0/1105	0.67	1/1477 (0.1%)
15	YT	0.35	0/1097	0.63	1/1468 (0.1%)
16	RU	0.32	0/977	0.55	0/1301
16	YU	0.37	0/977	0.54	0/1301

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
17	RV	0.35	0/786	0.57	0/1053
17	YV	0.37	0/782	0.61	0/1049
18	RW	0.35	0/897	0.57	0/1205
18	YW	0.37	0/897	0.57	0/1205
19	RX	0.39	0/764	0.59	0/1025
19	YX	0.39	0/764	0.61	0/1025
20	RY	0.34	0/823	0.64	0/1099
20	YY	0.39	0/823	0.63	0/1100
21	RZ	0.33	0/1620	0.55	0/2200
21	YZ	0.35	0/1590	0.59	0/2162
22	R0	0.39	0/616	0.70	1/821 (0.1%)
22	Y0	0.42	0/616	0.77	2/821 (0.2%)
23	R1	0.37	0/761	0.59	0/1013
23	Y1	0.38	0/766	0.64	0/1018
24	R2	0.29	0/590	0.50	0/781
24	Y2	0.35	0/594	0.54	0/785
25	R3	0.35	0/474	0.59	0/635
25	Y3	0.36	0/469	0.58	0/630
26	R4	0.37	0/559	0.70	0/754
26	Y4	0.40	0/549	0.70	1/741 (0.1%)
27	R5	0.44	0/473	0.64	0/639
27	Y5	0.41	0/469	0.60	0/635
28	R6	0.30	0/460	0.54	0/613
28	Y6	0.30	0/456	0.53	0/608
29	R7	0.40	0/426	0.67	0/561
29	Y7	0.42	0/426	0.69	0/561
30	R8	0.38	0/525	0.61	0/691
30	Y8	0.39	0/525	0.61	0/691
31	R9	0.32	0/310	0.68	0/407
31	Y9	0.33	0/310	0.68	0/407
32	QA	0.34	0/35795	0.88	12/55864 (0.0%)
32	XA	0.36	1/35890 (0.0%)	0.90	29/56012 (0.1%)
33	QB	0.34	0/1876	0.59	0/2533
33	XB	0.34	0/1860	0.60	1/2518 (0.0%)
34	QC	0.30	0/1582	0.53	0/2137
34	XC	0.36	1/1566 (0.1%)	0.61	0/2119
35	QD	0.33	0/1695	0.59	1/2274 (0.0%)
35	XD	0.32	0/1698	0.57	0/2277
36	QE	0.34	0/1149	0.55	0/1548
36	XE	0.32	0/1149	0.57	1/1548 (0.1%)
37	QF	0.31	0/827	0.55	0/1120
37	XF	0.33	0/829	0.64	1/1123 (0.1%)
38	QG	0.31	0/1254	0.46	0/1683

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
38	XG	0.31	0/1248	0.51	0/1676
39	QH	0.30	0/1118	0.53	0/1506
39	XH	0.32	0/1108	0.58	1/1494 (0.1%)
40	QI	0.32	0/1005	0.60	1/1351 (0.1%)
40	XI	0.31	0/985	0.54	0/1329
41	QJ	0.28	0/732	0.51	0/993
41	XJ	0.29	0/723	0.52	0/984
42	QK	0.30	0/849	0.55	0/1150
42	XK	0.30	0/848	0.57	0/1149
43	QL	0.39	0/937	0.61	0/1260
43	XL	0.36	0/937	0.67	0/1260
44	QM	0.30	0/924	0.57	0/1242
44	XM	0.31	0/905	0.55	0/1217
45	QN	0.34	0/501	0.59	1/664 (0.2%)
45	XN	0.35	0/501	0.58	0/664
46	QO	0.32	0/739	0.52	0/985
46	XO	0.35	0/739	0.56	0/985
47	QP	0.32	0/697	0.54	0/939
47	XP	0.30	0/693	0.57	0/935
48	QQ	0.33	0/836	0.55	0/1117
48	XQ	0.32	0/836	0.54	0/1117
49	QR	0.31	0/560	0.54	0/746
49	XR	0.32	0/560	0.59	0/746
50	QS	0.29	0/663	0.58	1/895 (0.1%)
50	XS	0.27	0/660	0.54	0/893
51	QT	0.31	0/734	0.51	0/969
51	XT	0.29	0/736	0.47	0/976
52	QU	0.30	0/203	0.58	0/266
52	XU	0.31	0/203	0.70	0/266
53	QV	0.34	0/1832	0.92	0/2855
53	XV	0.42	1/1836 (0.1%)	0.91	2/2859 (0.1%)
54	QX	0.39	0/216	0.83	0/334
54	XX	0.46	0/241	0.92	0/373
55	QY	0.36	0/2046	0.65	1/2759 (0.0%)
55	XY	0.40	0/2054	0.69	2/2770 (0.1%)
All	All	0.41	5/316497 (0.0%)	0.90	304/472893 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
14	RS	0	1
33	QB	0	1
43	XL	0	1
55	QY	0	1
All	All	0	4

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	XV	1	C	OP3-P	-10.47	1.48	1.61
32	XA	68	G	O3'-P	-6.54	1.53	1.61
34	XC	173	VAL	C-N	6.47	1.46	1.34
10	YO	21	CYS	CB-SG	-5.52	1.72	1.81
1	YA	1046	A	N3-C4	-5.10	1.31	1.34

All (304) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	YA	277	C	N1-C2-O2	17.75	129.55	118.90
1	YA	210	C	C6-N1-C2	12.43	125.27	120.30
1	YA	277	C	N3-C2-O2	-11.59	113.79	121.90
1	YA	277	C	N3-C4-N4	-11.48	109.96	118.00
1	YA	277	C	C5-C4-N4	10.97	127.88	120.20
1	YA	1083	U	N3-C4-O4	10.39	126.67	119.40
1	YA	210	C	N3-C4-C5	10.22	125.99	121.90
1	YA	1046	A	C5-C6-N1	-9.13	113.14	117.70
32	XA	1158	C	N1-C2-O2	8.82	124.19	118.90
32	XA	1158	C	C2-N1-C1'	8.07	127.68	118.80
1	YA	203	C	N1-C2-O2	7.83	123.59	118.90
1	YA	635	C	C6-N1-C2	-7.82	117.17	120.30
22	R0	11	ARG	NE-CZ-NH1	-7.79	116.41	120.30
1	RA	1097	U	C2-N1-C1'	7.74	126.99	117.70
1	YA	966	G	N1-C6-O6	-7.61	115.33	119.90
1	YA	512	G	O4'-C1'-N9	7.40	114.12	108.20
1	YA	966	G	C5-C6-O6	7.20	132.92	128.60
1	YA	2516	G	C5-C6-O6	-7.17	124.30	128.60
32	XA	266	G	P-O3'-C3'	7.17	128.30	119.70
1	RA	1092	C	N1-C2-O2	7.17	123.20	118.90
1	YA	277	C	C2-N3-C4	7.15	123.47	119.90
1	YA	12	U	N3-C2-O2	-7.13	117.21	122.20
55	XY	353	LEU	CA-CB-CG	7.12	131.67	115.30
1	YA	1372	U	N1-C2-O2	7.06	127.74	122.80
1	YA	1083	U	C6-N1-C2	-7.04	116.77	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	Y0	11	ARG	NE-CZ-NH1	7.03	123.82	120.30
1	YA	2506	U	C5-C4-O4	7.01	130.11	125.90
1	YA	676	A	C8-N9-C4	7.01	108.60	105.80
32	XA	1183	A	P-O3'-C3'	6.98	128.07	119.70
1	YA	813	U	N3-C2-O2	-6.97	117.32	122.20
1	YA	2463	C	N1-C2-O2	-6.94	114.74	118.90
1	YA	1820	U	N3-C2-O2	-6.90	117.37	122.20
1	RA	1640	C	C6-N1-C2	-6.87	117.55	120.30
1	YA	1625	C	N3-C4-N4	-6.86	113.20	118.00
1	YA	12	U	N1-C2-O2	6.86	127.60	122.80
1	YA	2751	G	N1-C6-O6	-6.86	115.78	119.90
32	XA	758	G	N1-C6-O6	6.85	124.01	119.90
1	YA	2506	U	N3-C2-O2	-6.78	117.45	122.20
1	YA	1083	U	N3-C4-C5	-6.76	110.55	114.60
8	YI	75	LEU	CA-CB-CG	6.75	130.83	115.30
15	RT	111	ARG	NE-CZ-NH1	6.73	123.67	120.30
1	YA	783	A	C8-N9-C4	-6.70	103.12	105.80
1	YA	2201	C	C6-N1-C2	6.70	122.98	120.30
1	YA	628	G	N1-C6-O6	-6.70	115.88	119.90
1	RA	1097	U	N3-C2-O2	-6.67	117.53	122.20
1	RA	799	G	N1-C6-O6	6.66	123.90	119.90
39	XH	14	ARG	NE-CZ-NH1	-6.66	116.97	120.30
32	XA	1158	C	N3-C2-O2	-6.64	117.25	121.90
5	RF	168	ARG	NE-CZ-NH1	6.61	123.61	120.30
1	RA	1097	U	N1-C2-O2	6.57	127.40	122.80
1	YA	1190	G	N1-C6-O6	-6.55	115.97	119.90
53	XV	13	C	C6-N1-C2	-6.54	117.68	120.30
1	YA	1369	G	N1-C6-O6	-6.51	116.00	119.90
1	YA	2435	A	N1-C6-N6	-6.51	114.70	118.60
1	YA	989	G	C5-C6-O6	-6.49	124.70	128.60
1	YA	974	G	C5-C6-O6	-6.49	124.71	128.60
55	QY	99	LEU	CA-CB-CG	6.48	130.21	115.30
1	YA	2237	G	C8-N9-C4	-6.47	103.81	106.40
1	YA	2440	C	O5'-P-OP2	-6.46	99.89	105.70
1	YA	1049	C	N1-C2-O2	6.43	122.76	118.90
22	Y0	11	ARG	NE-CZ-NH2	-6.42	117.09	120.30
32	QA	1030(C)	C	N1-C2-O2	6.42	122.75	118.90
1	YA	2554	U	O5'-P-OP1	-6.41	99.93	105.70
1	YA	2571	C	C6-N1-C2	6.39	122.86	120.30
5	RF	168	ARG	NE-CZ-NH2	-6.39	117.11	120.30
1	YA	1672	C	C6-N1-C2	6.37	122.85	120.30
1	YA	1097	U	C2-N1-C1'	6.36	125.33	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	YA	1611	C	C6-N1-C2	6.33	122.83	120.30
1	YA	1097	U	N1-C2-O2	6.32	127.23	122.80
1	YA	2242	G	O5'-P-OP1	-6.32	100.02	105.70
1	RA	1934	C	N1-C2-O2	6.31	122.69	118.90
1	YA	2047	U	N1-C2-O2	6.29	127.20	122.80
32	XA	1054	C	C6-N1-C2	-6.26	117.79	120.30
1	YA	1992	G	P-O3'-C3'	6.25	127.20	119.70
1	YA	2253	G	N1-C6-O6	6.24	123.64	119.90
32	XA	754	C	C2-N1-C1'	6.24	125.66	118.80
55	XY	100	LEU	CA-CB-CG	6.22	129.61	115.30
1	YA	1097	U	N3-C2-O2	-6.22	117.85	122.20
32	QA	115	G	P-O3'-C3'	6.20	127.14	119.70
32	QA	1030(C)	C	C2-N1-C1'	6.19	125.61	118.80
1	YA	277	C	P-O3'-C3'	6.19	127.13	119.70
1	YA	2501	C	C2-N1-C1'	-6.18	112.00	118.80
1	YA	2385	C	N3-C4-C5	6.18	124.37	121.90
1	RA	832	G	N1-C6-O6	-6.17	116.20	119.90
1	YA	2385	C	C6-N1-C2	6.17	122.77	120.30
1	RA	2386	C	C6-N1-C2	6.14	122.76	120.30
32	XA	1003	G	C4-N9-C1'	6.13	134.47	126.50
1	RA	778	G	C5-C6-O6	6.12	132.27	128.60
32	XA	1003	G	N3-C4-C5	-6.12	125.54	128.60
2	YB	6	C	C6-N1-C2	6.12	122.75	120.30
1	RA	1092	C	N3-C2-O2	-6.11	117.63	121.90
1	RA	1092	C	C2-N1-C1'	6.10	125.51	118.80
15	YT	111	ARG	NE-CZ-NH1	-6.10	117.25	120.30
1	YA	2524	G	N1-C6-O6	-6.08	116.25	119.90
1	YA	2569	G	N1-C6-O6	6.08	123.55	119.90
1	YA	1780	A	N1-C6-N6	-6.07	114.96	118.60
1	YA	1046	A	C6-N1-C2	6.07	122.24	118.60
1	RA	1940	U	N1-C2-O2	-6.06	118.56	122.80
1	YA	2573	C	N3-C4-N4	-6.06	113.76	118.00
1	RA	2445	G	N1-C6-O6	-6.04	116.28	119.90
1	YA	1083	U	C2-N1-C1'	6.02	124.92	117.70
32	XA	1183	A	OP1-P-O3'	6.01	118.43	105.20
32	XA	1003	G	C8-N9-C4	-5.99	104.00	106.40
1	YA	1530	C	P-O3'-C3'	5.98	126.88	119.70
1	YA	1806	C	C6-N1-C2	5.97	122.69	120.30
1	YA	203	C	N3-C4-N4	-5.97	113.82	118.00
4	YE	52	LEU	CA-CB-CG	5.97	129.03	115.30
1	RA	1045	A	P-O3'-C3'	5.97	126.86	119.70
32	QA	1442(A)	G	P-O3'-C3'	5.95	126.83	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	RA	728	G	N1-C6-O6	-5.92	116.35	119.90
1	YA	2699	C	N1-C2-O2	-5.91	115.35	118.90
1	RA	778	G	N1-C6-O6	-5.89	116.36	119.90
1	YA	1270	C	C6-N1-C2	5.88	122.65	120.30
1	YA	1811	G	C8-N9-C4	5.88	108.75	106.40
7	RH	69	ARG	NE-CZ-NH1	-5.87	117.36	120.30
1	YA	1046	A	N1-C6-N6	5.86	122.12	118.60
1	YA	1372	U	N3-C2-O2	-5.85	118.11	122.20
1	YA	209	C	C5-C4-N4	-5.84	116.11	120.20
1	YA	573	G	C8-N9-C4	-5.84	104.06	106.40
1	RA	744	G	N1-C6-O6	5.81	123.39	119.90
32	XA	1158	C	C6-N1-C1'	-5.78	113.86	120.80
1	RA	1530	C	P-O3'-C3'	5.78	126.64	119.70
1	YA	779	U	N3-C4-O4	5.77	123.44	119.40
1	YA	2047	U	N3-C2-O2	-5.76	118.17	122.20
1	RA	277	C	N1-C2-O2	5.75	122.35	118.90
7	YH	88	LEU	CA-CB-CG	5.75	128.51	115.30
1	YA	679	C	C6-N1-C2	5.74	122.60	120.30
1	RA	2061	G	N1-C6-O6	-5.72	116.47	119.90
1	YA	805	G	C5-C6-O6	-5.72	125.17	128.60
1	YA	1082	U	C5-C4-O4	-5.71	122.47	125.90
32	XA	803	G	C5-C6-O6	5.71	132.02	128.60
1	YA	1769	G	C2-N3-C4	5.70	114.75	111.90
1	YA	1854	A	C8-N9-C4	5.69	108.08	105.80
32	QA	943	U	P-O3'-C3'	5.69	126.53	119.70
3	YD	242	ARG	CG-CD-NE	5.68	123.74	111.80
26	Y4	60	GLN	N-CA-C	5.68	126.33	111.00
1	RA	1992	G	P-O3'-C3'	5.67	126.51	119.70
1	YA	2509	G	N3-C4-N9	5.67	129.40	126.00
1	YA	2056	G	N3-C4-N9	5.66	129.40	126.00
1	YA	1670	C	C5-C6-N1	5.65	123.82	121.00
1	YA	2385	C	C2-N3-C4	-5.65	117.08	119.90
1	RA	799	G	C5-C6-O6	-5.65	125.21	128.60
1	YA	2561	A	N1-C6-N6	5.64	121.98	118.60
32	QA	991	U	OP2-P-O3'	5.64	117.60	105.20
1	RA	2028	U	N1-C2-N3	5.63	118.28	114.90
1	YA	1625	C	N1-C2-O2	5.63	122.28	118.90
1	RA	2700	C	C6-N1-C2	5.62	122.55	120.30
32	XA	1003	G	N7-C8-N9	5.62	115.91	113.10
1	YA	2083	G	N1-C6-O6	5.62	123.27	119.90
1	RA	1092	C	C6-N1-C2	-5.61	118.05	120.30
1	YA	2501	C	C6-N1-C2	5.60	122.54	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	YA	2573	C	C6-N1-C2	5.60	122.54	120.30
1	RA	512	G	O4'-C1'-N9	5.59	112.68	108.20
1	YA	1046	A	C2-N3-C4	-5.59	107.81	110.60
1	RA	847	U	C2-N1-C1'	5.58	124.39	117.70
1	YA	2036	C	C6-N1-C2	-5.58	118.07	120.30
1	YA	2237	G	N9-C4-C5	5.57	107.63	105.40
1	YA	198	C	N3-C4-N4	-5.56	114.11	118.00
1	YA	210	C	C5-C6-N1	-5.55	118.22	121.00
1	YA	2689	U	P-O3'-C3'	5.55	126.36	119.70
1	YA	277	C	OP1-P-O3'	5.53	117.36	105.20
1	YA	1092	C	N1-C2-O2	5.52	122.21	118.90
1	YA	2496	C	C6-N1-C2	5.52	122.51	120.30
1	YA	1369	G	C5-C6-O6	5.52	131.91	128.60
1	YA	765	G	N1-C6-O6	-5.52	116.59	119.90
1	YA	2072	G	C5-C6-O6	5.52	131.91	128.60
1	YA	1798	U	N3-C4-O4	-5.51	115.54	119.40
1	RA	1789	A	C8-N9-C4	5.51	108.00	105.80
1	YA	579	G	N1-C6-O6	5.51	123.21	119.90
1	RA	1640	C	C5-C6-N1	5.50	123.75	121.00
1	RA	1277	G	C8-N9-C4	5.50	108.60	106.40
1	YA	2571	C	C5-C6-N1	-5.50	118.25	121.00
1	YA	278	A	O5'-P-OP1	-5.50	100.75	105.70
1	YA	1048	A	N1-C6-N6	-5.50	115.30	118.60
1	RA	436	C	N3-C2-O2	-5.49	118.06	121.90
1	YA	1083	U	C4-C5-C6	5.49	123.00	119.70
32	XA	284	G	N1-C6-O6	-5.49	116.61	119.90
1	YA	1092	C	C2-N1-C1'	5.49	124.84	118.80
32	XA	963	G	N1-C6-O6	-5.49	116.61	119.90
1	YA	128	C	C6-N1-C2	5.48	122.49	120.30
1	YA	746	A	O4'-C1'-N9	5.47	112.58	108.20
1	YA	678	C	C6-N1-C2	5.47	122.49	120.30
1	YA	1670	C	C6-N1-C2	-5.46	118.11	120.30
1	YA	1218	C	C6-N1-C2	5.45	122.48	120.30
1	YA	1083	U	N3-C2-O2	-5.45	118.39	122.20
1	YA	1063	G	C4-N9-C1'	5.43	133.56	126.50
32	XA	1067	A	P-O3'-C3'	5.43	126.22	119.70
1	YA	1807	G	C2-N3-C4	-5.43	109.19	111.90
1	RA	673	C	C6-N1-C2	-5.42	118.13	120.30
1	YA	624	C	C6-N1-C2	5.42	122.47	120.30
1	YA	2509	G	N3-C4-C5	-5.41	125.89	128.60
1	YA	1041	C	N1-C2-O2	5.41	122.14	118.90
1	YA	2569	G	C5-C6-O6	-5.41	125.36	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	YA	2004	G	C5-C6-O6	5.40	131.84	128.60
1	YA	692	C	C6-N1-C2	5.39	122.45	120.30
1	RA	1210	A	P-O3'-C3'	5.38	126.15	119.70
36	XE	143	ARG	NE-CZ-NH2	-5.37	117.62	120.30
1	YA	2247	A	C2-N3-C4	-5.36	107.92	110.60
32	XA	1054	C	C2-N1-C1'	5.36	124.70	118.80
32	XA	266	G	OP2-P-O3'	5.36	116.99	105.20
1	YA	974	G	N1-C6-O6	5.35	123.11	119.90
50	QS	28	LYS	CB-CA-C	-5.34	99.71	110.40
1	YA	531	C	N1-C2-O2	-5.34	115.70	118.90
1	RA	672	C	N1-C2-O2	5.33	122.10	118.90
1	RA	585	G	C6-C5-N7	-5.33	127.20	130.40
1	RA	1940	U	N3-C4-O4	5.33	123.13	119.40
1	RA	1763	G	C8-N9-C4	5.33	108.53	106.40
1	YA	1328	G	C5-C6-O6	-5.33	125.40	128.60
32	QA	839	U	P-O3'-C3'	5.32	126.08	119.70
1	YA	1313	U	C2-N1-C1'	5.32	124.08	117.70
1	YA	2447	G	C2-N3-C4	-5.31	109.25	111.90
1	YA	1091	G	N3-C4-C5	-5.31	125.95	128.60
1	YA	2072	G	N1-C6-O6	-5.31	116.72	119.90
1	RA	122	G	C8-N9-C4	5.31	108.52	106.40
1	YA	226	G	O4'-C1'-N9	5.30	112.44	108.20
1	YA	862	G	N1-C6-O6	-5.30	116.72	119.90
1	YA	678	C	O5'-P-OP2	-5.30	100.93	105.70
37	XF	82	ARG	NE-CZ-NH1	5.30	122.95	120.30
1	RA	388	G	C6-C5-N7	5.29	133.57	130.40
32	QA	1030(C)	C	N3-C2-O2	-5.29	118.20	121.90
32	XA	748	C	P-O3'-C3'	5.28	126.04	119.70
32	XA	1065	U	P-O3'-C3'	5.27	126.03	119.70
1	RA	778	G	C4-C5-N7	-5.27	108.69	110.80
32	QA	1419	G	N1-C6-O6	5.27	123.06	119.90
1	YA	2272	U	N3-C2-O2	5.27	125.89	122.20
32	XA	115	G	P-O3'-C3'	5.26	126.01	119.70
1	YA	966	G	N3-C2-N2	5.26	123.58	119.90
1	YA	132	G	C8-N9-C4	5.25	108.50	106.40
1	YA	2226	C	C6-N1-C2	5.25	122.40	120.30
1	YA	2070	G	C8-N9-C4	5.25	108.50	106.40
32	XA	1442(A)	G	P-O3'-C3'	5.25	126.00	119.70
1	YA	2506	U	N3-C4-O4	-5.25	115.73	119.40
1	RA	2751	G	C2-N3-C4	5.24	114.52	111.90
1	YA	1049	C	N3-C2-O2	-5.24	118.23	121.90
1	YA	1083	U	C5-C4-O4	-5.23	122.76	125.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	RA	585	G	N1-C6-O6	5.23	123.04	119.90
35	QD	13	ARG	NE-CZ-NH1	5.22	122.91	120.30
40	QI	42	ARG	NE-CZ-NH2	-5.22	117.69	120.30
1	RA	1790	C	N3-C4-C5	5.22	123.99	121.90
1	YA	2081	C	N1-C2-O2	5.22	122.03	118.90
1	YA	123	G	N1-C6-O6	5.21	123.03	119.90
1	RA	1082	U	C2-N1-C1'	5.20	123.94	117.70
32	XA	803	G	N1-C6-O6	-5.20	116.78	119.90
32	XA	1004	A	O4'-C1'-N9	5.20	112.36	108.20
33	XB	144	ARG	NE-CZ-NH1	-5.20	117.70	120.30
1	YA	2237	G	C5-C6-O6	5.19	131.72	128.60
1	YA	949	C	N3-C2-O2	5.18	125.53	121.90
1	YA	1314	C	C2-N1-C1'	5.17	124.49	118.80
1	YA	400	G	N1-C6-O6	5.17	123.00	119.90
32	XA	916	G	N1-C6-O6	-5.16	116.80	119.90
32	XA	766	A	C8-N9-C4	5.16	107.86	105.80
1	RA	1323	U	N3-C2-O2	5.15	125.81	122.20
3	RD	242	ARG	NE-CZ-NH1	5.15	122.88	120.30
1	YA	2689	U	N3-C2-O2	-5.15	118.59	122.20
1	YA	822	U	N3-C2-O2	-5.15	118.59	122.20
1	YA	2056	G	N3-C4-C5	-5.15	126.03	128.60
1	YA	2751	G	C5-C6-O6	5.15	131.69	128.60
1	YA	2751	G	C6-C5-N7	5.15	133.49	130.40
1	RA	1993	U	O5'-P-OP1	-5.14	101.07	105.70
1	YA	989	G	N1-C6-O6	5.14	122.98	119.90
1	YA	2249	U	N1-C2-O2	5.13	126.39	122.80
1	YA	1092	C	C5-C6-N1	5.13	123.56	121.00
1	YA	1611	C	N3-C4-C5	5.13	123.95	121.90
1	YA	209	C	N3-C4-N4	5.13	121.59	118.00
1	YA	2441	C	N3-C4-N4	-5.13	114.41	118.00
1	YA	2087	G	N1-C6-O6	5.12	122.97	119.90
1	YA	2068	U	N1-C2-O2	-5.12	119.22	122.80
32	XA	773	G	N1-C6-O6	-5.12	116.83	119.90
1	RA	2029	G	N1-C6-O6	-5.12	116.83	119.90
1	YA	238	C	C6-N1-C2	5.12	122.35	120.30
1	RA	388	G	N3-C4-N9	-5.11	122.93	126.00
1	YA	2336	A	C5-C6-N1	5.10	120.25	117.70
1	RA	752	A	P-O3'-C3'	5.10	125.82	119.70
1	RA	1636	C	C6-N1-C2	5.09	122.33	120.30
1	YA	791	C	C6-N1-C2	5.08	122.33	120.30
1	YA	1085	A	C2-N3-C4	5.08	113.14	110.60
1	YA	115	C	C5-C4-N4	-5.08	116.64	120.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	YA	214	G	O4'-C1'-N9	5.08	112.26	108.20
1	YA	667	U	N3-C4-O4	5.08	122.95	119.40
1	RA	775	G	N1-C6-O6	-5.07	116.86	119.90
1	YA	748	G	N3-C2-N2	-5.07	116.35	119.90
1	YA	783	A	C4-C5-C6	5.06	119.53	117.00
53	XV	53	G	P-O3'-C3'	5.06	125.77	119.70
1	YA	784	A	O4'-C1'-N9	5.06	112.25	108.20
1	YA	2318	G	C4-N9-C1'	5.06	133.07	126.50
32	QA	266	G	P-O3'-C3'	5.05	125.76	119.70
1	RA	2029	G	C6-C5-N7	5.05	133.43	130.40
1	YA	742	G	N1-C6-O6	5.05	122.93	119.90
1	YA	2440	C	N3-C4-C5	-5.05	119.88	121.90
1	YA	2525	G	C8-N9-C4	5.05	108.42	106.40
1	YA	2571	C	N3-C4-C5	5.04	123.92	121.90
32	QA	1285	A	P-O3'-C3'	5.04	125.75	119.70
1	YA	832	G	P-O3'-C3'	5.03	125.74	119.70
1	YA	2495	G	C8-N9-C4	5.03	108.41	106.40
32	QA	791	G	N3-C2-N2	-5.02	116.39	119.90
1	YA	1125	G	C5-C6-O6	5.02	131.61	128.60
1	YA	1671	U	C5-C4-O4	-5.02	122.89	125.90
1	RA	2751	G	N1-C2-N2	5.01	120.71	116.20
45	QN	31	ARG	NE-CZ-NH2	-5.01	117.79	120.30
1	YA	2509	G	C2-N3-C4	5.01	114.41	111.90
1	YA	2692	C	N3-C2-O2	-5.01	118.39	121.90
1	YA	622	G	C8-N9-C4	5.01	108.40	106.40
1	RA	2075	U	O5'-P-OP1	-5.01	101.19	105.70
1	YA	1602	U	N1-C2-O2	-5.00	119.30	122.80

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
33	QB	231	GLU	Peptide
55	QY	305	ASP	Peptide
14	RS	58	LEU	Peptide
43	XL	86	ARG	Peptide

## 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	RA	61758	0	31144	585	0
1	YA	61758	0	31147	606	1
2	RB	2572	0	1305	11	0
2	YB	2573	0	1306	12	0
3	RD	2131	0	2207	49	0
3	YD	2136	0	2218	49	0
4	RE	1559	0	1618	34	0
4	YE	1559	0	1618	40	0
5	RF	1584	0	1625	37	0
5	YF	1580	0	1619	46	0
6	RG	1426	0	1445	30	0
6	YG	1424	0	1441	38	0
7	RH	1330	0	1407	20	0
7	YH	1324	0	1402	33	0
8	RI	1094	0	1127	22	0
8	YI	1076	0	1093	14	0
9	RN	1121	0	1195	16	0
9	YN	1117	0	1184	16	0
10	RO	933	0	996	17	0
10	YO	933	0	996	14	0
11	RP	1135	0	1212	22	0
11	YP	1135	0	1212	32	0
12	RQ	1122	0	1179	20	0
12	YQ	1122	0	1179	20	0
13	RR	968	0	1033	21	0
13	YR	968	0	1033	13	0
14	RS	877	0	938	12	0
14	YS	870	0	923	13	0
15	RT	1091	0	1151	25	0
15	YT	1083	0	1136	19	0
16	RU	959	0	1019	16	0
16	YU	959	0	1019	18	0
17	RV	775	0	841	13	0
17	YV	771	0	830	13	0
18	RW	886	0	940	12	0
18	YW	886	0	940	12	0
19	RX	750	0	814	16	0
19	YX	750	0	814	6	0
20	RY	810	0	894	15	0
20	YY	810	0	891	17	0
21	RZ	1587	0	1598	24	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	YZ	1557	0	1564	24	0
22	R0	608	0	622	12	0
22	Y0	608	0	622	15	0
23	R1	754	0	823	10	0
23	Y1	759	0	837	18	0
24	R2	588	0	643	11	1
24	Y2	592	0	654	7	0
25	R3	469	0	518	5	0
25	Y3	464	0	514	6	0
26	R4	546	0	523	27	0
26	Y4	536	0	516	26	0
27	R5	459	0	477	12	0
27	Y5	455	0	467	5	0
28	R6	453	0	475	7	0
28	Y6	449	0	471	7	0
29	R7	418	0	467	11	0
29	Y7	418	0	467	8	0
30	R8	517	0	582	17	0
30	Y8	517	0	582	19	0
31	R9	307	0	336	14	0
31	Y9	307	0	336	11	0
32	QA	32246	0	16294	307	0
32	XA	32331	0	16338	343	0
33	QB	1842	0	1862	54	0
33	XB	1825	0	1828	62	0
34	QC	1558	0	1557	33	0
34	XC	1542	0	1517	32	0
35	QD	1665	0	1690	60	0
35	XD	1668	0	1706	44	0
36	QE	1133	0	1191	28	0
36	XE	1133	0	1191	25	0
37	QF	814	0	808	20	0
37	XF	816	0	807	8	0
38	QG	1235	0	1249	18	0
38	XG	1229	0	1238	15	0
39	QH	1098	0	1143	20	0
39	XH	1088	0	1126	21	0
40	QI	986	0	990	28	0
40	XI	966	0	953	35	0
41	QJ	719	0	672	27	0
41	XJ	710	0	661	20	0
42	QK	834	0	838	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
42	XK	833	0	836	13	0
43	QL	932	0	981	18	0
43	XL	932	0	981	26	0
44	QM	914	0	954	23	0
44	XM	895	0	920	24	0
45	QN	492	0	529	11	0
45	XN	492	0	529	14	0
46	QO	728	0	760	12	0
46	XO	728	0	760	13	0
47	QP	681	0	697	19	0
47	XP	677	0	686	19	0
48	QQ	823	0	891	8	0
48	XQ	823	0	891	9	0
49	QR	555	0	618	11	0
49	XR	555	0	618	9	0
50	QS	648	0	658	17	0
50	XS	645	0	635	19	0
51	QT	732	0	809	15	0
51	XT	733	0	795	13	0
52	QU	199	0	208	3	0
52	XU	199	0	208	1	0
53	QV	1640	0	837	15	0
53	XV	1644	0	836	15	0
54	QX	193	0	98	5	0
54	XX	215	0	108	2	0
55	QY	2014	0	1980	73	0
55	XY	2022	0	1991	85	0
56	QA	262	0	0	0	0
56	QB	1	0	0	0	0
56	QD	2	0	0	0	0
56	QE	2	0	0	0	0
56	QF	1	0	0	0	0
56	QG	3	0	0	0	0
56	QH	1	0	0	0	0
56	QI	1	0	0	0	0
56	QJ	1	0	0	0	0
56	QL	2	0	0	0	0
56	QN	1	0	0	0	0
56	QO	1	0	0	0	0
56	QQ	1	0	0	0	0
56	QR	1	0	0	0	0
56	QT	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	QV	6	0	0	0	0
56	R0	7	0	0	0	0
56	R1	5	0	0	0	0
56	R3	2	0	0	0	0
56	R5	1	0	0	0	0
56	R7	3	0	0	0	0
56	R9	1	0	0	0	0
56	RA	1032	0	0	0	0
56	RB	22	0	0	0	0
56	RD	15	0	0	0	0
56	RE	7	0	0	0	0
56	RF	11	0	0	0	0
56	RG	4	0	0	0	0
56	RN	2	0	0	0	0
56	RO	1	0	0	0	0
56	RP	2	0	0	0	0
56	RQ	5	0	0	0	0
56	RR	4	0	0	0	0
56	RS	1	0	0	0	0
56	RT	3	0	0	0	0
56	RU	3	0	0	0	0
56	RV	3	0	0	0	0
56	RW	2	0	0	0	0
56	RX	1	0	0	0	0
56	RY	1	0	0	0	0
56	XA	187	0	0	0	0
56	XE	2	0	0	0	0
56	XF	4	0	0	0	0
56	XJ	1	0	0	0	0
56	XL	1	0	0	0	0
56	XT	1	0	0	0	0
56	XV	4	0	0	0	0
56	XY	1	0	0	0	0
56	Y0	1	0	0	0	0
56	Y1	1	0	0	0	0
56	Y5	2	0	0	0	0
56	Y7	1	0	0	0	0
56	Y8	2	0	0	0	0
56	YA	749	0	0	0	0
56	YB	20	0	0	0	0
56	YD	9	0	0	0	0
56	YE	6	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	YF	2	0	0	0	0
56	YG	2	0	0	0	0
56	YI	1	0	0	0	0
56	YN	1	0	0	0	0
56	YO	1	0	0	0	0
56	YP	1	0	0	0	0
56	YQ	3	0	0	0	0
56	YR	1	0	0	0	0
56	YT	3	0	0	0	0
56	YV	1	0	0	0	0
56	YW	2	0	0	0	0
56	YX	1	0	0	0	0
57	QN	1	0	0	0	0
57	R4	1	0	0	0	0
57	R5	1	0	0	0	0
57	R6	1	0	0	0	0
57	R9	1	0	0	0	0
57	RY	1	0	0	0	0
57	XN	1	0	0	0	0
57	Y4	1	0	0	0	0
57	Y5	1	0	0	0	0
57	Y6	1	0	0	0	0
57	Y9	1	0	0	0	0
57	YY	1	0	0	0	0
58	QD	8	0	0	0	0
58	XD	8	0	0	0	0
All	All	294929	0	198658	3416	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (3416) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:RA:2552:2MU:C5	1:RA:2552:2MU:C4	1.74	1.65
1:YA:2552:2MU:C4	1:YA:2552:2MU:C5	1.75	1.56
32:XA:1003:G:H2'	32:XA:1004:A:H4'	1.40	1.03
1:YA:2131:G:H5''	1:YA:2132:U:H5'	1.46	0.98
26:Y4:59:PHE:HA	26:Y4:61:ARG:H	1.26	0.97
1:RA:2131:G:H5''	1:RA:2132:U:H5'	1.45	0.96
15:RT:55:ASN:H	15:RT:59:THR:HG22	1.30	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:Y4:59:PHE:HA	26:Y4:61:ARG:N	1.80	0.96
33:QB:82:ARG:NH1	33:QB:92:TYR:OH	2.01	0.93
12:RQ:21:THR:HG21	12:RQ:101:ARG:HB2	1.52	0.92
55:XY:242:SER:HA	55:XY:263:GLN:HB3	1.53	0.90
35:QD:3:ARG:HD3	35:QD:118:ARG:HE	1.37	0.89
29:Y7:34:ARG:HG2	29:Y7:39:ARG:HG3	1.53	0.89
14:RS:59:LYS:HD2	14:RS:60:GLY:H	1.37	0.89
1:YA:2552:2MU:C4	1:YA:2552:2MU:C6	2.48	0.88
8:YI:92:VAL:HG23	8:YI:120:ILE:HB	1.56	0.88
1:YA:2785:C:OP1	4:YE:41:LYS:NZ	2.08	0.87
10:YO:48:PRO:HB3	32:XA:1422:G:H5''	1.57	0.86
7:RH:7:LEU:O	7:RH:69:ARG:NH1	2.09	0.85
55:XY:212:ALA:HB1	55:XY:214:LEU:HG	1.59	0.85
55:QY:242:SER:HA	55:QY:263:GLN:HB3	1.59	0.84
40:QI:17:VAL:HG21	40:QI:81:ILE:HG22	1.60	0.84
33:QB:231:GLU:HB3	33:QB:232:PRO:HD3	1.58	0.83
33:XB:15:VAL:HB	33:XB:209:ARG:HB3	1.60	0.83
10:RO:35:VAL:HG11	10:RO:103:ALA:HB3	1.62	0.82
21:YZ:198:LYS:HE3	53:XV:52:G:H2'	1.61	0.82
55:QY:123:GLU:HG3	55:QY:188:PRO:HB3	1.59	0.82
1:YA:301:G:OP2	20:YY:84:ARG:NH2	2.13	0.82
32:XA:664:G:H22	32:XA:741:G:H1	1.27	0.82
1:RA:143(A):G:H4'	19:RX:35:THR:HG21	1.60	0.81
32:QA:1103:C:OP1	33:QB:96:ARG:NH2	2.12	0.81
5:YF:10:PRO:HB3	5:YF:17:ARG:HE	1.45	0.81
15:YT:65:LYS:HE3	15:YT:67:SER:HB2	1.62	0.81
32:QA:78:G:H1	32:QA:91:C:H42	1.27	0.81
3:YD:17:THR:O	3:YD:211:ARG:NH2	2.14	0.80
1:RA:2573:C:N4	55:QY:239:THR:HA	1.96	0.80
1:YA:2573:C:N4	55:XY:239:THR:O	2.13	0.80
32:QA:343:U:O2'	32:QA:346:G:O6	2.00	0.80
55:XY:101:LEU:HD11	55:XY:353:LEU:HD23	1.62	0.80
41:QJ:35:SER:HB3	41:QJ:73:ASP:HB2	1.63	0.80
1:RA:2529:G:O6	31:R9:31:LYS:NZ	2.14	0.80
32:XA:582:U:OP1	46:XO:68:ARG:NH2	2.14	0.80
32:XA:1398:A:OP1	55:XY:193:GLN:NE2	2.15	0.80
32:XA:559:A:OP1	36:XE:126:ARG:NH2	2.14	0.79
1:YA:631:A:OP1	11:YP:65:ARG:NH1	2.14	0.79
41:XJ:49:VAL:HG23	45:YN:41:ARG:HB2	1.64	0.79
1:RA:987:G:O2'	1:RA:1000:A:N3	2.16	0.79
50:XS:50:ALA:HB1	50:XS:57:HIS:HB3	1.64	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:YA:1798:U:H5'	3:YD:259:THR:HG22	1.63	0.79
42:XK:99:GLN:HG2	42:XK:105:VAL:HG21	1.63	0.79
1:RA:833:U:O2	11:RP:55:ARG:NH2	2.15	0.78
29:R7:24:THR:HG23	29:R7:27:GLY:H	1.48	0.78
1:RA:2140:C:H2'	1:RA:2141:G:H8	1.49	0.78
10:RO:48:PRO:HB3	32:QA:1422:G:H5''	1.64	0.78
1:RA:1798:U:OP2	3:RD:274:ARG:NH2	2.17	0.78
1:RA:1048:A:N6	1:RA:2751:G:O6	2.17	0.78
1:YA:2128:C:H42	1:YA:2160:G:H1	1.32	0.77
40:XI:53:VAL:O	40:XI:55:ALA:N	2.17	0.77
10:YO:35:VAL:HG11	10:YO:103:ALA:HB3	1.65	0.77
55:XY:263:GLN:O	55:XY:267:LYS:N	2.17	0.77
6:RG:179:PRO:HB2	26:R4:42:PHE:HE2	1.49	0.77
1:RA:250:G:OP2	30:R8:13:ARG:NH2	2.18	0.77
1:RA:1057:A:N6	1:RA:1087:G:OP1	2.17	0.77
55:QY:102:PRO:HG3	55:QY:353:LEU:HD21	1.65	0.77
1:RA:2478:A:OP2	31:R9:2:LYS:NZ	2.17	0.77
1:YA:2469:A:O2'	12:YQ:56:ARG:NH1	2.17	0.77
1:RA:1041:C:H42	1:RA:1114:G:H1	1.31	0.77
1:RA:1141:U:OP1	9:RN:25:ARG:NH1	2.18	0.77
32:XA:390:C:O3'	47:XP:28:ARG:NH2	2.18	0.77
1:RA:2128:C:H42	1:RA:2160:G:H1	1.30	0.76
53:XV:75:C:OP2	55:XY:261:ARG:NH2	2.17	0.76
22:R0:10:THR:HG22	22:R0:12:ASN:H	1.50	0.76
11:YP:59:LEU:HD11	30:Y8:10:ALA:HB2	1.66	0.76
32:QA:1189:C:OP1	41:QJ:51:ARG:NH2	2.19	0.76
1:YA:1048:A:N6	1:YA:2751:G:O6	2.18	0.76
32:XA:975:A:H4'	32:XA:976:G:H5''	1.67	0.76
32:XA:401:C:OP2	35:XD:73:ARG:NH2	2.15	0.76
23:Y1:51:VAL:HG11	23:Y1:74:VAL:HG21	1.68	0.76
1:RA:1530:C:O2'	1:RA:1531:C:O5'	2.03	0.76
6:YG:113:ARG:HH21	26:Y4:33:VAL:HG12	1.51	0.76
1:RA:2552:2MU:C4	1:RA:2552:2MU:C6	2.49	0.76
55:XY:214:LEU:HB2	55:XY:215:PRO:HA	1.67	0.76
20:RY:92:ASN:HB2	20:RY:94:LYS:H	1.51	0.76
4:YE:47:VAL:HG11	4:YE:86:PRO:HD2	1.67	0.76
19:RX:60:ARG:HH22	29:R7:47:ARG:HH22	1.31	0.75
5:RF:53:THR:HG22	5:RF:55:GLY:H	1.51	0.75
11:RP:59:LEU:HD11	30:R8:10:ALA:HB2	1.68	0.75
55:QY:209:LEU:O	55:QY:211:ASP:N	2.19	0.75
29:R7:34:ARG:NH1	29:R7:41:ARG:O	2.19	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:QB:15:VAL:HG23	33:QB:209:ARG:HB3	1.68	0.75
1:YA:574:C:N3	4:YE:145:LYS:NZ	2.34	0.75
33:XB:17:PHE:HD1	33:XB:18:GLY:H	1.35	0.75
32:XA:1310:G:OP2	44:XM:88:ARG:NH1	2.19	0.75
1:RA:1038:C:H42	1:RA:1117:G:H1	1.34	0.75
4:RE:47:VAL:HG21	4:RE:86:PRO:HD2	1.67	0.75
32:XA:677:U:H3	32:XA:713:G:H22	1.33	0.75
20:RY:102:CYS:SG	20:RY:103:GLY:N	2.59	0.74
1:YA:250:G:OP2	30:Y8:13:ARG:NH2	2.21	0.74
1:RA:2285:C:OP1	28:R6:29:ASN:ND2	2.20	0.74
1:YA:587:C:OP2	11:YP:21:ARG:NH2	2.20	0.74
33:QB:21:ARG:HH22	33:QB:23:ARG:HE	1.35	0.74
1:YA:2285:C:OP2	28:Y6:26:ASN:ND2	2.18	0.74
26:Y4:59:PHE:CE1	50:XS:64:GLU:HB2	2.23	0.74
5:YF:178:PRO:HB2	5:YF:201:VAL:HG21	1.68	0.74
48:XQ:66:SER:O	48:XQ:70:ARG:NH1	2.21	0.74
6:RG:139:LEU:HD21	6:RG:149:VAL:HG11	1.70	0.73
3:RD:69:ARG:HG2	3:RD:69:ARG:HH11	1.53	0.73
21:YZ:144:LEU:HD21	21:YZ:150:LEU:HD13	1.69	0.73
33:XB:88:ALA:HB1	33:XB:222:ILE:HD11	1.70	0.73
1:YA:1971:A:OP2	3:YD:242:ARG:NH2	2.20	0.73
32:QA:201:C:H42	32:QA:216:G:H1	1.36	0.73
34:XC:40:ARG:NH2	34:XC:55:VAL:O	2.19	0.73
47:QP:53:VAL:HG13	47:QP:79:VAL:HG12	1.70	0.73
55:XY:217:ILE:HD12	55:XY:222:LEU:HD11	1.69	0.73
1:YA:2134:A:N6	1:YA:2156:G:O2'	2.22	0.73
1:RA:2746:U:OP1	7:RH:85:LYS:NZ	2.22	0.72
32:QA:677:U:H3	32:QA:713:G:H22	1.33	0.72
40:QI:121:ARG:NH1	40:QI:122:ALA:O	2.22	0.72
32:QA:975:A:H4'	32:QA:976:G:H5''	1.70	0.72
32:QA:1352:C:OP1	52:QU:3:LYS:NZ	2.21	0.72
35:QD:53:ASP:HB3	35:QD:57:ARG:HH12	1.54	0.72
31:Y9:16:VAL:HG22	31:Y9:25:VAL:HG22	1.72	0.72
32:XA:1518:MA6:H93	32:XA:1519:MA6:H102	1.71	0.72
40:XI:16:ARG:HB2	40:XI:64:THR:HG22	1.71	0.72
1:RA:2206:G:H3'	1:RA:2207:G:C8	2.25	0.72
33:QB:88:ALA:O	33:QB:226:ARG:NH2	2.21	0.72
1:YA:270:A:OP2	1:YA:272(X):G:N1	2.20	0.72
6:RG:161:THR:HG22	6:RG:163:ALA:H	1.55	0.72
1:RA:463:G:N2	1:RA:466:A:OP2	2.20	0.72
44:XM:58:GLU:O	44:XM:62:ASN:ND2	2.21	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:YA:1359:A:H61	1:YA:1372:U:H3	1.38	0.72
1:YA:2140:C:H2'	1:YA:2141:G:H8	1.53	0.72
8:YI:9:LEU:HD12	8:YI:12:LEU:HD12	1.72	0.72
1:YA:1530:C:O2'	1:YA:1531:C:O5'	2.06	0.72
1:YA:1593:G:H2'	1:YA:1594:G:C8	2.25	0.72
20:YY:102:CYS:SG	20:YY:103:GLY:N	2.63	0.72
32:QA:38:G:H22	32:QA:397:A:H5'	1.55	0.72
1:RA:631:A:OP1	11:RP:65:ARG:NH1	2.23	0.71
5:YF:18:ARG:HG2	5:YF:19:GLU:H	1.54	0.71
44:XM:107:ALA:HB3	44:XM:111:LYS:HD2	1.71	0.71
51:XT:56:MET:HE1	51:XT:85:MET:HG2	1.72	0.71
34:XC:58:GLU:HB3	41:XJ:92:THR:HG21	1.70	0.71
44:QM:19:LEU:HD21	44:QM:56:LEU:HD21	1.73	0.71
11:YP:2:LYS:NZ	11:YP:4:SER:OG	2.23	0.71
55:XY:123:GLU:OE1	55:XY:199:SER:OG	2.07	0.71
22:R0:23:VAL:HG22	22:R0:38:VAL:HG22	1.70	0.71
1:YA:1815:A:OP2	3:YD:54:ARG:NH2	2.24	0.71
32:XA:642:A:N3	39:XH:113:SER:OG	2.23	0.71
33:XB:128:GLU:OE1	33:XB:135:GLN:NE2	2.21	0.70
55:XY:245:ARG:HG3	55:XY:256:GLU:HG2	1.71	0.70
1:YA:1064:C:H3'	1:YA:1065:U:H5'	1.72	0.70
21:RZ:158:PRO:HG2	21:RZ:161:VAL:HG11	1.74	0.70
36:QE:126:ARG:HH11	36:QE:126:ARG:HG3	1.57	0.70
32:XA:1360:A:OP2	45:YN:35:ARG:NH2	2.25	0.70
50:QS:50:ALA:HB1	50:QS:57:HIS:HB3	1.73	0.70
1:YA:1041:C:H42	1:YA:1114:G:H1	1.39	0.70
13:YR:96:ARG:NH1	13:YR:115:GLU:OE1	2.24	0.70
36:QE:79:GLU:HG3	36:QE:93:PRO:HD2	1.73	0.70
32:QA:538:G:H5''	43:QL:114:LYS:HB2	1.74	0.70
11:YP:86:LYS:HB3	11:YP:118:GLY:HA3	1.74	0.70
32:QA:1003:G:N2	32:QA:1004:A:N3	2.39	0.70
55:QY:328:ARG:HD2	55:QY:340:LEU:HD21	1.72	0.70
1:YA:1798:U:OP2	3:YD:274:ARG:NH2	2.24	0.70
1:YA:1914:C:C2	55:XY:295:ARG:HD3	2.27	0.70
32:XA:1292:U:OP2	38:XG:41:ARG:NH2	2.24	0.70
55:XY:255:VAL:HG12	55:XY:274:LEU:HG	1.73	0.70
26:R4:57:GLU:HB2	26:R4:58:ARG:HA	1.72	0.70
32:QA:1360:A:OP2	45:QN:35:ARG:NH2	2.24	0.70
6:RG:41:GLN:HB3	6:RG:43:LEU:HD13	1.73	0.69
32:XA:696:A:N1	32:XA:797:C:O2'	2.22	0.69
1:RA:2785:C:OP1	4:RE:41:LYS:NZ	2.24	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:QA:189(B):C:H42	32:QA:189(K):G:H1	1.39	0.69
55:QY:114:GLU:HB2	55:QY:204:ALA:HB3	1.74	0.69
1:YA:2640:G:O3'	9:YN:74:ARG:NH2	2.19	0.69
32:XA:474:G:H2'	32:XA:475:G:H8	1.56	0.69
32:XA:427:U:OP1	35:XD:13:ARG:NH2	2.25	0.69
41:XJ:17:ASP:OD1	41:XJ:70:ARG:NH1	2.25	0.69
22:Y0:11:ARG:O	22:Y0:14:ARG:NH2	2.25	0.69
36:XE:50:GLU:HB2	36:XE:53:LEU:HD13	1.74	0.69
6:YG:161:THR:HG22	6:YG:163:ALA:H	1.56	0.69
1:RA:652(C):A:H61	1:RA:655:A:H1'	1.57	0.69
1:RA:1071:G:N2	1:RA:1089:G:O6	2.17	0.69
1:RA:1378:A:OP1	29:R7:10:ARG:NH2	2.26	0.69
40:QI:50:LEU:HD13	40:QI:56:LEU:HA	1.72	0.69
13:YR:67:LEU:HD13	13:YR:76:VAL:HG21	1.75	0.69
15:YT:16:ARG:NH2	15:YT:83:ILE:O	2.26	0.69
1:RA:1009:A:OP2	9:RN:37:LYS:NZ	2.24	0.69
1:RA:2748:A:H5'	7:RH:4:ILE:HD12	1.75	0.69
1:YA:2748:A:H5'	7:YH:4:ILE:HD12	1.74	0.69
44:QM:3:ARG:HD2	44:QM:9:ILE:HG12	1.75	0.68
4:YE:12:THR:HG23	15:YT:58:ASN:HD21	1.56	0.68
32:XA:486:U:H2'	32:XA:487:A:H8	1.57	0.68
50:XS:41:VAL:HG12	50:XS:44:MET:HG3	1.74	0.68
1:YA:1071:G:N2	1:YA:1089:G:O6	2.18	0.68
27:R5:16:ARG:NH1	27:R5:17:ASP:OD1	2.26	0.68
32:QA:571:U:O4	32:QA:864:A:N6	2.26	0.68
36:XE:69:VAL:HG11	36:XE:113:ALA:HB1	1.75	0.68
55:XY:101:LEU:H	55:XY:103:LYS:HE3	1.57	0.68
35:QD:173:TRP:CD2	35:QD:189:PRO:HG3	2.28	0.68
33:XB:91:PRO:HG3	33:XB:155:LEU:HD23	1.76	0.68
40:XI:46:ALA:HB2	40:XI:74:ILE:HG23	1.76	0.68
47:QP:13:HIS:O	47:QP:42:ARG:NH1	2.27	0.68
1:RA:1817:G:OP1	3:RD:88:ARG:NH2	2.26	0.68
6:YG:41:GLN:HB3	6:YG:43:LEU:HD13	1.74	0.68
32:XA:1412:C:H2'	32:XA:1413:A:C8	2.29	0.68
33:QB:195:ASP:O	39:QH:68:ARG:NH2	2.27	0.68
33:QB:185:ILE:HG22	33:QB:199:TYR:HB2	1.75	0.68
38:QG:113:GLU:HG2	38:QG:119:ARG:HG2	1.76	0.68
46:QO:7:GLU:OE2	46:QO:38:ARG:NH2	2.26	0.68
4:YE:52:LEU:HB3	4:YE:53:PRO:HD2	1.74	0.68
32:XA:1278:U:H5''	32:XA:1279:A:H5'	1.74	0.68
5:RF:18:ARG:HG2	5:RF:19:GLU:H	1.58	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:YA:2206:G:H5''	1:YA:2207:G:C8	2.28	0.67
34:XC:152:ILE:HG12	34:XC:199:LYS:HB2	1.76	0.67
33:QB:19:HIS:NE2	33:QB:189:ASP:OD2	2.27	0.67
33:XB:187:LEU:HA	33:XB:201:ILE:HB	1.75	0.67
9:RN:46:VAL:HG23	9:RN:48:MET:HG2	1.77	0.67
1:YA:11:G:H2'	1:YA:12:U:H5'	1.76	0.67
1:YA:2206:G:H3'	1:YA:2207:G:H8	1.58	0.67
41:XJ:61:GLU:OE1	45:YN:58:LYS:NZ	2.27	0.67
5:RF:51:THR:HB	5:RF:88:VAL:HG11	1.77	0.67
15:RT:55:ASN:N	15:RT:59:THR:HG22	2.06	0.67
32:QA:664:G:H22	32:QA:741:G:H1	1.42	0.67
6:YG:143:GLU:OE2	26:Y4:26:SER:OG	2.10	0.67
22:Y0:10:THR:HG22	22:Y0:12:ASN:H	1.60	0.67
32:XA:978:A:O2'	32:XA:1322:C:N3	2.27	0.67
6:RG:143:GLU:OE2	26:R4:26:SER:OG	2.12	0.67
8:RI:109:ILE:HG13	8:RI:130:TYR:CZ	2.30	0.67
35:QD:23:GLY:N	35:QD:26:CYS:SG	2.68	0.67
1:YA:1639:U:H2'	1:YA:1640:C:H5''	1.76	0.67
32:XA:1223:C:OP1	50:XS:78:ARG:NH2	2.27	0.67
1:RA:956:G:OP2	12:RQ:14:ARG:NH2	2.27	0.67
26:R4:50:VAL:HG11	44:QM:65:LYS:HA	1.76	0.66
1:RA:2206:G:H3'	1:RA:2207:G:H8	1.60	0.66
27:R5:40:LYS:HD3	27:R5:46:CYS:HA	1.77	0.66
37:QF:15:ASP:OD1	37:QF:18:GLN:N	2.25	0.66
1:YA:517:C:OP1	27:Y5:16:ARG:NH2	2.28	0.66
1:YA:987:G:O2'	1:YA:1000:A:N3	2.29	0.66
32:XA:559:A:H4'	32:XA:560:U:H3'	1.78	0.66
32:XA:64:G:H4'	32:XA:65:U:H3'	1.77	0.66
28:Y6:35:GLU:OE2	28:Y6:50:ARG:NH1	2.28	0.66
34:XC:152:ILE:HD11	34:XC:199:LYS:HD2	1.78	0.66
3:RD:71:ASP:HB3	3:RD:103:ARG:HH22	1.61	0.66
21:RZ:144:LEU:HD21	21:RZ:150:LEU:HD13	1.76	0.66
1:RA:1063:G:N2	1:RA:1075:C:N3	2.43	0.66
1:RA:2576:G:O2'	1:RA:2579:C:OP2	2.11	0.66
6:RG:18:GLU:OE1	6:RG:21:ARG:NH1	2.28	0.66
23:R1:3:LYS:HG3	23:R1:4:VAL:H	1.60	0.66
1:YA:714:U:N3	1:YA:717:G:OP2	2.27	0.66
1:YA:2753:A:N3	31:Y9:15:LYS:NZ	2.37	0.66
1:RA:2355:C:H1'	22:R0:39:ARG:HH21	1.61	0.66
34:QC:114:PRO:O	34:QC:118:GLN:HG3	1.96	0.66
6:YG:21:ARG:HD3	6:YG:22:ARG:N	2.11	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:Y5:16:ARG:NH1	27:Y5:17:ASP:OD1	2.29	0.66
1:RA:2469:A:O2'	12:RQ:56:ARG:NH1	2.29	0.66
5:RF:165:ARG:HA	5:RF:168:ARG:HD2	1.78	0.66
43:QL:70:ILE:HG12	43:QL:100:ILE:HD12	1.77	0.66
3:YD:147:LEU:HD11	3:YD:183:ARG:HE	1.60	0.66
32:XA:976:G:H5'	32:XA:1358:U:O2'	1.96	0.66
35:XD:23:GLY:N	35:XD:26:CYS:SG	2.68	0.66
1:YA:2469:A:HO2'	12:YQ:56:ARG:HH11	1.44	0.65
32:XA:9:G:O5'	36:XE:126:ARG:NH1	2.29	0.65
32:XA:954:G:H21	32:XA:1227:A:H62	1.44	0.65
1:YA:637:A:H5''	11:YP:117:GLU:HG2	1.79	0.65
29:Y7:9:ARG:HH21	29:Y7:47:ARG:HD2	1.61	0.65
1:RA:2134:A:N6	1:RA:2156:G:O2'	2.29	0.65
38:QG:27:ILE:HD12	38:QG:40:ALA:HA	1.77	0.65
32:XA:1128:C:H1'	32:XA:1147:C:H42	1.60	0.65
32:QA:532:A:H61	34:QC:193:TYR:HA	1.61	0.65
16:YU:89:GLU:OE1	17:YV:50:PRO:HB3	1.97	0.65
27:Y5:40:LYS:NZ	27:Y5:44:THR:O	2.28	0.65
32:XA:1518:MA6:H93	32:XA:1519:MA6:C10	2.27	0.65
1:RA:2781:A:H5''	1:RA:2782:G:H5'	1.78	0.65
32:XA:1510:U:H2'	32:XA:1511:G:C8	2.31	0.65
39:XH:64:LYS:HG2	39:XH:79:VAL:HG21	1.78	0.65
1:RA:1667:G:O2'	1:RA:1991:U:O4	2.10	0.65
6:YG:136:ARG:HG2	6:YG:137:GLU:HG3	1.78	0.65
32:XA:1005:A:OP2	32:XA:1024:G:N2	2.30	0.65
55:XY:292:SER:O	55:XY:296:ASN:ND2	2.30	0.65
1:YA:334:C:OP1	1:YA:335:C:N4	2.30	0.65
32:XA:552:U:O3'	43:XL:87:GLY:HA2	1.96	0.65
5:YF:51:THR:HB	5:YF:88:VAL:HG11	1.79	0.65
26:Y4:61:ARG:HH22	50:XS:9:VAL:HG21	1.62	0.65
32:XA:1073:U:O2'	33:XB:104:ASN:OD1	2.13	0.65
1:RA:2357:U:OP1	22:R0:20:ARG:NH1	2.29	0.65
32:QA:922:G:H4'	36:QE:20:GLN:HA	1.78	0.65
34:QC:58:GLU:HB3	41:QJ:92:THR:HG21	1.77	0.65
41:QJ:52:GLY:O	45:QN:41:ARG:NH2	2.28	0.65
50:QS:41:VAL:HG12	50:QS:44:MET:HG3	1.78	0.65
26:Y4:59:PHE:HE1	50:XS:64:GLU:HB2	1.58	0.65
11:RP:63:PRO:HD3	30:R8:27:THR:HG22	1.78	0.64
55:QY:332:VAL:HG13	55:QY:337:LEU:HD22	1.79	0.64
32:XA:955:U:OP1	55:XY:137:ARG:NH2	2.30	0.64
1:RA:1069:A:H5'	1:RA:1096:A:H5'	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:QA:1030(A):C:N4	32:QA:1032:G:O6	2.30	0.64
3:YD:242:ARG:HD3	3:YD:242:ARG:H	1.62	0.64
1:RA:26:G:H1'	1:RA:515:A:H61	1.61	0.64
1:RA:309:G:N3	1:RA:329:G:O2'	2.29	0.64
32:QA:142:G:O2'	32:QA:196:A:N1	2.29	0.64
34:QC:40:ARG:O	34:QC:44:GLU:HB2	1.96	0.64
1:YA:307:G:N1	1:YA:310:A:OP2	2.31	0.64
32:XA:406:G:O2'	35:XD:3:ARG:NH2	2.31	0.64
41:QJ:61:GLU:OE2	45:QN:49:HIS:NE2	2.25	0.64
4:YE:11:MET:HG2	4:YE:24:THR:HG22	1.78	0.64
1:RA:1045:A:O2'	1:RA:1046:A:OP2	2.15	0.64
40:XI:32:ASP:HB3	40:XI:35:GLU:HB3	1.79	0.64
1:YA:143(A):G:H4'	19:YX:35:THR:HG21	1.80	0.64
9:YN:15:LEU:HB2	9:YN:135:PRO:HB2	1.79	0.64
32:XA:1070:U:OP1	36:XE:20:GLN:NE2	2.26	0.64
1:RA:582:G:H2'	1:RA:583:G:C8	2.33	0.64
32:QA:560:U:O2'	32:QA:561:U:OP2	2.14	0.64
1:YA:1786:A:H1'	1:YA:1938:A:N6	2.12	0.64
32:XA:974:A:OP2	45:YN:29:ARG:NH2	2.31	0.64
55:QY:245:ARG:HG3	55:QY:256:GLU:CD	2.17	0.64
44:XM:96:LEU:O	44:XM:110:ARG:NH1	2.31	0.64
15:RT:56:GLY:O	15:RT:59:THR:HG23	1.98	0.63
32:QA:707:C:OP1	42:QK:85:ARG:NH1	2.30	0.63
1:YA:997:G:OP1	16:YU:92:ARG:HG2	1.98	0.63
1:YA:2206:G:H3'	1:YA:2207:G:C8	2.33	0.63
35:XD:18:LYS:NZ	35:XD:31:CYS:SG	2.71	0.63
44:XM:17:VAL:O	44:XM:20:THR:OG1	2.11	0.63
51:XT:56:MET:CE	51:XT:85:MET:HG2	2.27	0.63
1:RA:102:G:OP1	24:R2:7:ARG:NH2	2.31	0.63
1:RA:1786:A:H1'	1:RA:1938:A:N6	2.13	0.63
32:QA:159:G:N2	32:QA:162:A:OP2	2.19	0.63
32:QA:316:G:OP2	32:QA:351:G:O2'	2.16	0.63
1:YA:2478:A:OP2	31:Y9:2:LYS:NZ	2.27	0.63
1:YA:2572:A:C8	4:YE:144:ARG:HD3	2.32	0.63
39:XH:10:LEU:HD22	39:XH:83:ILE:HD11	1.79	0.63
1:RA:321:G:OP1	5:RF:135:LYS:NZ	2.27	0.63
24:R2:16:LEU:O	24:R2:67:LYS:NZ	2.31	0.63
1:YA:652(C):A:H61	1:YA:655:A:H1'	1.64	0.63
1:YA:1500:G:O2'	3:YD:100:GLY:O	2.14	0.63
1:YA:1721:G:H8	1:YA:1741:A:H62	1.44	0.63
35:XD:175:SER:HB3	35:XD:186:LEU:HD11	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:QD:108:LEU:HD21	35:QD:183:GLY:HA3	1.80	0.63
41:QJ:49:VAL:HG23	45:QN:41:ARG:HB2	1.79	0.63
32:XA:687:A:O2'	32:XA:701:C:N4	2.30	0.63
31:R9:16:VAL:HG22	31:R9:25:VAL:HG22	1.79	0.63
36:QE:8:GLU:HG2	36:QE:34:VAL:HG22	1.80	0.63
1:RA:2223:G:OP1	3:RD:172:TYR:OH	2.16	0.63
18:RW:14:PRO:HG2	18:RW:78:GLU:HG3	1.81	0.63
6:YG:16:ARG:HE	6:YG:31:VAL:HG21	1.64	0.63
11:YP:138:LEU:HD23	11:YP:145:PRO:HB3	1.80	0.63
32:XA:316:G:OP2	32:XA:351:G:O2'	2.15	0.63
32:QA:673:G:H2'	32:QA:674:G:C8	2.34	0.63
1:YA:851:U:O2'	25:Y3:42:ALA:O	2.14	0.63
1:YA:956:G:OP2	12:YQ:14:ARG:NH2	2.32	0.63
32:XA:501:C:OP1	43:XL:117:ARG:NH2	2.32	0.63
15:RT:24:PRO:HA	15:RT:49:VAL:HG23	1.80	0.63
32:QA:791:G:N2	32:QA:1497:G:O3'	2.31	0.63
1:RA:336:C:O2'	20:RY:35:TYR:OH	2.16	0.63
1:RA:1064:C:H3'	1:RA:1065:U:H5'	1.80	0.63
1:YA:2156:G:N7	1:YA:2157:G:N2	2.47	0.63
55:XY:108:GLU:HA	55:XY:170:GLY:HA2	1.81	0.63
55:XY:136:SER:HA	55:XY:146:VAL:HG21	1.81	0.63
1:RA:1087:G:N2	1:RA:1102:C:N3	2.37	0.62
1:YA:1491:G:O2'	3:YD:101:GLU:HB2	1.99	0.62
11:YP:63:PRO:HG2	30:Y8:25:MET:HB2	1.81	0.62
32:QA:1310:G:OP2	44:QM:88:ARG:NH1	2.31	0.62
33:QB:118:LEU:HB3	33:QB:142:LEU:HD13	1.81	0.62
36:QE:69:VAL:HG11	36:QE:113:ALA:HB1	1.80	0.62
55:QY:296:ASN:O	55:QY:306:ARG:NH1	2.32	0.62
1:YA:637:A:H8	11:YP:117:GLU:HG3	1.64	0.62
1:YA:1823:G:OP1	3:YD:54:ARG:NH1	2.32	0.62
1:RA:1064:C:H3'	1:RA:1065:U:C5'	2.30	0.62
1:RA:2285:C:OP2	28:R6:26:ASN:ND2	2.31	0.62
1:YA:1063:G:N2	1:YA:1075:C:N3	2.48	0.62
1:YA:2807:G:N1	1:YA:2893:G:O6	2.31	0.62
4:YE:12:THR:HG22	4:YE:13:ARG:H	1.63	0.62
32:QA:78:G:H1	32:QA:91:C:N4	1.96	0.62
1:RA:1019:U:OP1	1:RA:1035:U:O2'	2.17	0.62
1:YA:2619:C:OP1	4:YE:152:LYS:NZ	2.28	0.62
7:YH:7:LEU:O	7:YH:69:ARG:NH1	2.33	0.62
1:RA:2424:C:O2	1:RA:2429:G:O2'	2.13	0.62
32:QA:1239:A:O2'	38:QG:114:ARG:O	2.13	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:QY:138:TYR:CE1	55:QY:338:ASP:HB3	2.35	0.62
1:YA:1113:U:O2'	1:YA:1114:G:H8	1.82	0.62
32:QA:974:A:OP2	45:QN:29:ARG:NH2	2.33	0.62
43:QL:117:ARG:HG2	43:QL:122:THR:HB	1.81	0.62
32:XA:552:U:H4'	43:XL:86:ARG:HD3	1.81	0.62
32:XA:1492:A:H5'	43:XL:47:LYS:HE2	1.81	0.62
1:RA:2390:U:P	30:R8:35:GLN:HE22	2.22	0.62
1:RA:2572:A:N7	4:RE:144:ARG:HD2	2.15	0.62
12:RQ:32:TYR:OH	12:RQ:111:GLU:OE1	2.17	0.62
33:QB:16:HIS:HB2	33:QB:204:ASN:HB3	1.81	0.62
4:YE:119:ARG:HG3	4:YE:160:TYR:HB2	1.82	0.62
40:XI:50:LEU:HD23	40:XI:85:LEU:HD11	1.80	0.62
1:RA:307:G:N1	1:RA:310:A:OP2	2.32	0.61
1:RA:1971:A:OP2	3:RD:242:ARG:NH2	2.32	0.61
10:RO:64:ARG:NE	10:RO:101:PRO:O	2.31	0.61
18:RW:4:LYS:HB2	18:RW:106:ILE:HG12	1.82	0.61
32:QA:1097:C:O2'	32:QA:1169:A:N3	2.27	0.61
46:QO:16:ALA:HB1	46:QO:21:ASP:HB3	1.81	0.61
1:RA:1568:G:H5''	3:RD:61:LEU:HD13	1.81	0.61
35:QD:55:ALA:O	35:QD:59:ARG:HG2	2.00	0.61
32:XA:662:G:H2'	32:XA:663:A:C8	2.36	0.61
32:XA:1103:C:OP1	33:XB:96:ARG:NH2	2.33	0.61
33:XB:101:MET:HA	33:XB:108:ILE:HG13	1.81	0.61
33:XB:118:LEU:HB3	33:XB:142:LEU:HD12	1.81	0.61
2:RB:66:A:H61	2:RB:109:C:H5''	1.65	0.61
42:QK:99:GLN:HG2	42:QK:105:VAL:HG21	1.83	0.61
35:XD:12:CYS:SG	35:XD:19:LEU:HB2	2.40	0.61
1:RA:1639:U:H2'	1:RA:1640:C:H5''	1.82	0.61
26:R4:59:PHE:HZ	50:QS:45:VAL:HG21	1.64	0.61
32:QA:1020:U:H2'	32:QA:1021:G:C8	2.36	0.61
1:YA:1049:C:H42	1:YA:2751:G:N2	1.98	0.61
11:YP:59:LEU:HD21	30:Y8:10:ALA:HA	1.82	0.61
53:XV:4:G:HO2'	53:XV:5:G:H8	1.48	0.61
1:RA:764:A:H5'	3:RD:210:GLY:HA2	1.81	0.61
1:YA:1038:C:H42	1:YA:1117:G:H1	1.47	0.61
1:YA:1086:A:OP1	1:YA:1104:C:O2'	2.18	0.61
1:YA:1641:A:H2'	1:YA:1642:G:O4'	2.00	0.61
6:YG:80:PHE:O	6:YG:82:LEU:N	2.33	0.61
46:QO:25:THR:HG21	46:QO:70:LEU:HB2	1.82	0.61
32:XA:1221:G:OP1	32:XA:1320:C:N4	2.31	0.61
33:XB:78:GLN:O	33:XB:94:ASN:ND2	2.30	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:XI:42:ARG:NH1	40:XI:71:SER:O	2.33	0.61
55:XY:340:LEU:O	55:XY:343:PRO:HD2	2.00	0.61
11:RP:99:LEU:HD23	11:RP:102:ARG:HH21	1.65	0.61
1:YA:1593:G:H2'	1:YA:1594:G:H8	1.66	0.61
1:YA:1889:A:N1	1:YA:2234:G:H1'	2.16	0.61
32:XA:1189:C:OP1	41:XJ:51:ARG:NH2	2.32	0.61
6:RG:101:ILE:HD13	26:R4:25:TYR:HB2	1.83	0.61
32:QA:126:G:OP1	32:QA:605:U:O2'	2.14	0.61
5:YF:164:ARG:HD2	5:YF:175:THR:HG23	1.83	0.61
24:R2:31:GLU:HB3	24:R2:53:LEU:HD11	1.82	0.61
44:QM:81:LEU:HD13	44:QM:88:ARG:HD2	1.82	0.61
1:YA:265:A:N1	1:YA:427:U:O2'	2.28	0.61
1:YA:1266:G:O5'	18:YW:15:ARG:NH2	2.34	0.61
33:XB:98:LEU:O	33:XB:101:MET:HG3	2.01	0.61
35:XD:65:ARG:NH2	35:XD:72:GLU:HB2	2.16	0.61
55:XY:123:GLU:HG2	55:XY:188:PRO:HB3	1.83	0.61
1:RA:212:G:H2'	1:RA:213:A:O4'	2.00	0.61
1:RA:2126:A:H4'	1:RA:2127:G:O5'	2.01	0.61
1:RA:2206:G:H5''	1:RA:2207:G:N7	2.16	0.61
50:QS:12:ASP:HB3	50:QS:14:HIS:CE1	2.36	0.61
3:YD:108:PRO:HB3	3:YD:143:HIS:CE1	2.35	0.61
18:YW:14:PRO:HG2	18:YW:78:GLU:CG	2.31	0.61
44:XM:3:ARG:HG3	44:XM:8:GLU:HG3	1.83	0.61
49:XR:32:ARG:HA	49:XR:69:THR:HG21	1.83	0.61
13:RR:67:LEU:HD13	13:RR:76:VAL:HG21	1.83	0.60
32:XA:992:U:H4'	32:XA:993:G:O5'	2.00	0.60
51:XT:50:GLU:HG3	51:XT:100:ILE:HD11	1.83	0.60
1:YA:2130:U:H2'	1:YA:2158:A:H61	1.66	0.60
1:YA:2327:A:H2'	1:YA:2328:A:C8	2.35	0.60
12:YQ:34:LEU:HB2	12:YQ:118:LEU:HD22	1.83	0.60
1:RA:577:G:O2'	1:RA:1254:A:OP1	2.19	0.60
1:YA:1651:G:H5'	13:YR:39:PRO:HG2	1.82	0.60
30:Y8:6:THR:HG22	30:Y8:63:PRO:HD2	1.84	0.60
38:XG:15:ASP:OD1	38:XG:20:ASP:N	2.29	0.60
55:QY:247:THR:HA	55:QY:254:VAL:HG12	1.83	0.60
7:YH:27:LYS:HD3	7:YH:32:GLU:HB2	1.82	0.60
1:RA:1053:C:H2'	1:RA:1054:A:H8	1.66	0.60
8:RI:54:GLN:HG3	8:RI:57:ARG:HH11	1.67	0.60
9:RN:67:LEU:HD12	9:RN:87:LEU:HD13	1.83	0.60
34:XC:57:ILE:HG12	34:XC:66:VAL:HG22	1.84	0.60
4:RE:78:LEU:O	4:RE:79:ARG:NH1	2.30	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:YA:1507:A:O2'	1:YA:1508:A:O5'	2.18	0.60
1:YA:1657:C:H2'	1:YA:1658:C:C6	2.37	0.60
5:YF:184:TYR:CE2	5:YF:188:ARG:HD2	2.37	0.60
11:YP:50:ARG:HD3	30:Y8:7:HIS:CD2	2.37	0.60
16:YU:89:GLU:O	17:YV:11:GLN:NE2	2.34	0.60
23:R1:50:ARG:HG2	23:R1:59:THR:HG22	1.83	0.60
35:QD:162:LEU:HD13	35:QD:181:MET:HG2	1.82	0.60
1:YA:83:G:N2	1:YA:103:A:OP2	2.35	0.60
13:YR:36:THR:HG22	13:YR:37:THR:H	1.65	0.60
32:XA:359:U:H2'	32:XA:360:A:C8	2.37	0.60
36:XE:102:ALA:HB1	36:XE:106:PRO:HG2	1.82	0.60
37:QF:23:LYS:HG2	37:QF:61:LEU:HD21	1.84	0.60
1:YA:2218:U:O2	23:Y1:52:ARG:NH2	2.35	0.60
23:Y1:53:VAL:HG22	23:Y1:74:VAL:HG13	1.83	0.60
5:RF:157:VAL:HB	5:RF:194:MET:HG2	1.82	0.60
25:Y3:10:LYS:NZ	25:Y3:15:TYR:OH	2.30	0.60
55:XY:245:ARG:HG3	55:XY:256:GLU:CG	2.32	0.60
32:QA:269:C:H2'	32:QA:270:A:C8	2.37	0.60
32:XA:1316:G:N1	32:XA:1319:A:OP2	2.33	0.60
33:XB:229:VAL:HG12	33:XB:230:VAL:H	1.67	0.60
34:XC:8:ILE:HG23	34:XC:16:ARG:HD3	1.82	0.60
20:RY:92:ASN:N	20:RY:93:GLY:HA2	2.16	0.59
7:YH:87:LEU:HD23	7:YH:164:TYR:HA	1.83	0.59
32:XA:537:G:H5''	43:XL:113:ARG:NH1	2.17	0.59
33:XB:18:GLY:HA2	33:XB:42:ILE:HD12	1.84	0.59
7:RH:3:ARG:HD3	7:RH:54:ARG:HH12	1.66	0.59
21:RZ:19:ARG:NH1	21:RZ:84:GLU:O	2.35	0.59
28:R6:9:LEU:HD13	28:R6:51:GLU:HG3	1.83	0.59
44:QM:15:VAL:HG11	44:QM:48:LEU:HD21	1.84	0.59
1:YA:1935:G:H3'	1:YA:1962:5MC:HN41	1.66	0.59
32:XA:17:U:H2'	32:XA:18:C:C6	2.36	0.59
33:XB:73:THR:OG1	33:XB:170:GLU:OE1	2.19	0.59
39:QH:86:ILE:HG13	39:QH:133:LEU:HD22	1.84	0.59
1:YA:1073:A:H2'	1:YA:1074:G:C8	2.36	0.59
1:YA:2552:2MU:O5'	1:YA:2552:2MU:H6	2.02	0.59
2:YB:14:U:OP2	2:YB:70:C:O2'	2.19	0.59
32:XA:790:A:OP1	53:XV:38:A:O2'	2.18	0.59
33:XB:185:ILE:HG13	33:XB:199:TYR:HB2	1.85	0.59
1:YA:1803:A:O2'	3:YD:259:THR:HG21	2.02	0.59
35:XD:122:ARG:NH1	35:XD:134:ASP:O	2.36	0.59
32:QA:1030(D):G:N7	32:QA:1031:G:N2	2.50	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:QV:15:G:N2	53:QV:21:A:N3	2.50	0.59
33:XB:47:THR:HA	33:XB:202:PRO:HG2	1.85	0.59
34:QC:8:ILE:HG23	34:QC:16:ARG:HD3	1.83	0.59
1:YA:2122:U:H3	1:YA:2176:A:H61	1.51	0.59
1:YA:2787:C:H1'	4:YE:62:PRO:HG3	1.85	0.59
21:YZ:198:LYS:NZ	53:XV:53:G:O4'	2.34	0.59
55:XY:151:ALA:HB2	55:XY:162:ILE:HD12	1.85	0.59
1:RA:2755:C:O2	31:R9:20:HIS:NE2	2.35	0.59
5:RF:167:ALA:HB1	5:RF:173:VAL:HG11	1.84	0.59
14:YS:27:SER:HA	14:YS:88:ASP:HB3	1.83	0.59
41:XJ:5:ARG:N	41:XJ:99:LYS:O	2.36	0.59
1:RA:1075:C:H2'	1:RA:1076:C:H5'	1.85	0.59
1:YA:1688:U:O2	1:YA:1700:A:H5'	2.03	0.59
23:Y1:76:ARG:HH22	23:Y1:97:LEU:HB3	1.66	0.59
36:XE:20:GLN:NE2	36:XE:25:ARG:HD2	2.17	0.59
8:RI:54:GLN:HG3	8:RI:57:ARG:NH1	2.18	0.59
32:QA:45:U:H2'	32:QA:46:G:C8	2.38	0.59
32:QA:524:G:H2'	32:QA:525:C:C6	2.37	0.59
43:QL:33:ARG:HH11	43:QL:62:SER:HB3	1.66	0.59
46:QO:39:LEU:HD13	46:QO:56:LEU:HB2	1.83	0.59
3:YD:71:ASP:HB3	3:YD:103:ARG:HH22	1.67	0.59
1:RA:2537:U:H2'	1:RA:2538:C:C6	2.38	0.59
35:QD:12:CYS:SG	35:QD:19:LEU:HB2	2.43	0.59
40:QI:16:ARG:HB2	40:QI:64:THR:HG22	1.83	0.59
1:YA:1794:U:H2'	1:YA:1795:C:H6	1.68	0.59
1:YA:2279:G:N7	22:Y0:14:ARG:NH1	2.51	0.59
26:Y4:16:CYS:SG	26:Y4:17:GLY:N	2.76	0.59
33:XB:166:ASP:HB3	33:XB:169:LYS:HB3	1.83	0.59
1:RA:994:C:OP1	16:RU:53:ARG:NH2	2.36	0.58
29:R7:12:ARG:NH2	29:R7:44:PRO:HB3	2.18	0.58
9:YN:96:GLU:HB2	9:YN:122:VAL:HG12	1.84	0.58
11:YP:100:LEU:HD12	11:YP:112:LEU:HD11	1.84	0.58
24:Y2:31:GLU:HB3	24:Y2:53:LEU:HD11	1.85	0.58
39:QH:64:LYS:HG2	39:QH:79:VAL:HG21	1.84	0.58
1:YA:616:G:H5'	5:YF:205:ARG:HD3	1.84	0.58
1:YA:796:C:H2'	1:YA:797:C:C6	2.39	0.58
7:YH:55:PRO:HG2	7:YH:61:HIS:CE1	2.37	0.58
9:YN:67:LEU:O	9:YN:88:GLU:HG3	2.03	0.58
32:XA:1182:G:H4'	32:XA:1183:A:H3'	1.85	0.58
32:XA:1314:C:OP2	50:XS:4:SER:OG	2.12	0.58
38:XG:113:GLU:HG2	38:XG:119:ARG:HG2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:RA:192:C:O2'	1:RA:802:A:N3	2.30	0.58
1:RA:2312:U:H5'	6:RG:88:ILE:HD11	1.85	0.58
1:RA:2619:C:OP1	4:RE:152:LYS:NZ	2.33	0.58
18:RW:14:PRO:HG2	18:RW:78:GLU:CG	2.32	0.58
32:QA:692:U:O2'	32:QA:694:A:N7	2.32	0.58
35:QD:85:LYS:HD3	35:QD:86:LYS:H	1.68	0.58
1:YA:286:C:H2'	1:YA:287:C:C6	2.38	0.58
1:YA:601:C:O2'	1:YA:605:C:OP1	2.20	0.58
5:YF:167:ALA:HB1	5:YF:173:VAL:HG11	1.85	0.58
32:XA:1244:C:H2'	32:XA:1245:A:C8	2.39	0.58
20:RY:102:CYS:SG	20:RY:104:GLY:N	2.67	0.58
1:YA:1073:A:H2'	1:YA:1074:G:H8	1.68	0.58
32:XA:539:A:H2'	32:XA:540:G:C8	2.38	0.58
1:RA:1073:A:H2'	1:RA:1074:G:C8	2.38	0.58
1:RA:1798:U:H5'	3:RD:259:THR:HG22	1.86	0.58
18:YW:14:PRO:HG2	18:YW:78:GLU:HG2	1.85	0.58
32:XA:890:G:O2'	32:XA:906:G:O6	2.17	0.58
32:XA:1047:G:H5''	45:YN:4:LYS:HD3	1.83	0.58
55:XY:330:ASP:O	55:XY:334:GLU:HB3	2.02	0.58
10:RO:64:ARG:NH2	10:RO:99:PHE:O	2.37	0.58
11:RP:63:PRO:HG2	30:R8:25:MET:HB2	1.84	0.58
15:RT:60:THR:HG22	15:RT:77:PRO:HA	1.86	0.58
35:QD:15:GLU:OE2	35:QD:59:ARG:NH2	2.20	0.58
13:YR:29:LEU:HB3	13:YR:75:LEU:HD21	1.86	0.58
32:XA:1116:C:H2'	32:XA:1117:G:H5''	1.86	0.58
32:XA:1318:A:H5''	50:XS:3:ARG:HH22	1.66	0.58
1:RA:1165:U:H2'	1:RA:1166:C:C6	2.38	0.58
1:RA:1266:G:O4'	18:RW:15:ARG:NH2	2.34	0.58
5:RF:24:LEU:HD23	5:RF:115:ALA:HA	1.85	0.58
21:RZ:203:GLU:CD	53:QV:54:U:H5''	2.24	0.58
26:R4:59:PHE:CZ	50:QS:45:VAL:HG21	2.38	0.58
32:QA:1309:G:N7	44:QM:99:ARG:NH2	2.50	0.58
32:QA:1391:U:H2'	32:QA:1392:G:C8	2.39	0.58
33:XB:114:ARG:NH1	33:XB:141:GLU:OE1	2.37	0.58
32:QA:1402:4OC:HM22	32:QA:1403:C:H5'	1.84	0.58
55:QY:346:GLN:O	55:QY:349:GLN:HG2	2.03	0.58
1:YA:78:A:H2'	1:YA:79:G:H8	1.68	0.58
1:YA:572:A:OP2	17:YV:78:LYS:NZ	2.34	0.58
1:YA:2115:G:N1	1:YA:2119:A:OP2	2.37	0.58
2:YB:14:U:O3'	2:YB:108:U:O2'	2.22	0.58
6:YG:15:VAL:HG21	6:YG:176:LEU:HD23	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:XK:117:ASN:OD1	42:XK:117:ASN:N	2.36	0.58
1:RA:674:G:H1'	5:RF:74:ARG:HD3	1.86	0.58
19:RX:60:ARG:NH2	29:R7:47:ARG:HH22	2.01	0.58
5:YF:185:ASP:HA	5:YF:188:ARG:HD3	1.86	0.58
6:YG:77:ILE:HG21	6:YG:80:PHE:CD2	2.39	0.58
42:XK:62:GLN:HB2	42:XK:93:GLN:HG3	1.86	0.58
35:QD:167:GLY:H	35:QD:168:ARG:NH2	2.02	0.58
32:XA:1031:G:H2'	32:XA:1032:G:C8	2.39	0.58
1:RA:198:C:H5'	1:RA:2244:U:OP1	2.04	0.57
15:RT:39:ARG:HH12	15:RT:41:ARG:HD3	1.67	0.57
44:QM:3:ARG:HG3	44:QM:4:ILE:H	1.69	0.57
1:YA:2115:G:H21	1:YA:2171:A:H61	1.53	0.57
20:YY:15:VAL:O	20:YY:22:GLY:N	2.26	0.57
32:XA:1343:G:H4'	40:XI:122:ALA:HB3	1.86	0.57
1:RA:1289:C:H2'	1:RA:1290:C:C6	2.39	0.57
32:QA:103:C:O2'	32:QA:172:A:N1	2.31	0.57
32:QA:1298:C:C4	38:QG:114:ARG:HD2	2.39	0.57
37:QF:36:ARG:NH2	37:QF:66:GLU:OE1	2.36	0.57
55:QY:204:ALA:HB2	55:QY:298:LEU:HD21	1.86	0.57
1:YA:1470:G:N2	1:YA:1520:G:OP2	2.32	0.57
41:XJ:35:SER:HB3	41:XJ:73:ASP:H	1.68	0.57
55:XY:226:THR:HG22	55:XY:244:ILE:HD12	1.86	0.57
1:RA:1936:A:OP2	1:RA:1962:5MC:N4	2.28	0.57
1:YA:36:G:N3	1:YA:450:G:O2'	2.35	0.57
1:YA:300:A:OP1	20:YY:86:ARG:NH2	2.36	0.57
32:XA:452:A:N3	47:XP:72:ARG:NH1	2.52	0.57
55:XY:214:LEU:HB2	55:XY:215:PRO:CA	2.35	0.57
1:RA:1507:A:O2'	1:RA:1508:A:O5'	2.19	0.57
1:RA:1800:C:OP1	3:RD:260:ARG:NH2	2.36	0.57
49:QR:32:ARG:HA	49:QR:69:THR:HG21	1.86	0.57
1:YA:2711:A:H5''	1:YA:2712(A):U:H5''	1.86	0.57
39:XH:14:ARG:O	39:XH:18:ARG:HG2	2.05	0.57
41:XJ:11:PHE:HE1	41:XJ:67:THR:HG22	1.69	0.57
1:RA:1289:C:H2'	1:RA:1290:C:H6	1.68	0.57
49:QR:29:PHE:HE1	49:QR:31:LEU:HD13	1.70	0.57
33:XB:77:ALA:HB2	33:XB:211:ILE:HD13	1.86	0.57
32:QA:1435:G:H2'	32:QA:1436:U:C6	2.40	0.57
53:XV:51:C:H2'	53:XV:52:G:O4'	2.04	0.57
1:RA:1062:G:H5'	1:RA:1070:A:H5''	1.85	0.57
1:YA:784:A:C6	3:YD:229:VAL:HG11	2.40	0.57
6:YG:11:TYR:HA	6:YG:15:VAL:HB	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:RA:482:A:O2'	1:RA:497:A:N1	2.35	0.57
1:RA:1252:G:N1	16:RU:37:GLU:OE1	2.37	0.57
3:RD:10:THR:OG1	3:RD:13:ARG:HG2	2.05	0.57
32:QA:1519:MA6:H8	32:QA:1519:MA6:O5'	2.04	0.57
32:XA:501:C:H2'	32:XA:502:G:C8	2.39	0.57
44:QM:32:GLU:HG2	44:QM:64:TRP:HZ2	1.70	0.57
44:QM:32:GLU:HG2	44:QM:64:TRP:CZ2	2.40	0.57
32:XA:201:C:H42	32:XA:216:G:H1	1.51	0.57
1:RA:2820:A:OP2	13:RR:2:ARG:NH2	2.38	0.57
7:RH:11:VAL:HG21	7:RH:50:VAL:HG23	1.86	0.57
32:QA:642:A:N3	39:QH:113:SER:OG	2.33	0.57
39:QH:6:ILE:HB	39:QH:85:ARG:NH1	2.20	0.57
1:YA:2233:U:H2'	1:YA:2234:G:C8	2.39	0.57
1:YA:2312:U:H5'	6:YG:88:ILE:HD11	1.86	0.57
32:XA:380:G:N2	32:XA:383:A:OP2	2.37	0.57
55:XY:145:ARG:HB2	55:XY:167:SER:OG	2.05	0.57
1:RA:958:U:OP2	12:RQ:14:ARG:NH1	2.37	0.56
32:QA:403:C:O2'	35:QD:122:ARG:NH1	2.38	0.56
32:QA:814:A:H2'	32:QA:816:A:H5''	1.86	0.56
1:YA:1064:C:H5''	1:YA:1065:U:H3'	1.87	0.56
3:YD:242:ARG:HD3	3:YD:242:ARG:N	2.20	0.56
5:YF:53:THR:HG22	5:YF:56:GLU:HG3	1.87	0.56
7:YH:86:GLU:OE2	7:YH:132:ARG:NH2	2.38	0.56
26:Y4:18:CYS:SG	26:Y4:39:CYS:HB3	2.45	0.56
1:RA:1796:U:H2'	1:RA:1797:C:C6	2.40	0.56
36:QE:33:VAL:HG21	36:QE:109:ILE:HA	1.86	0.56
1:YA:2150:U:H2'	1:YA:2151:G:C8	2.40	0.56
4:YE:34:VAL:HG12	4:YE:72:VAL:HG21	1.87	0.56
12:YQ:80:GLU:OE2	55:XY:264:HIS:CD2	2.58	0.56
34:XC:109:PRO:HB3	34:XC:115:LEU:HD23	1.87	0.56
55:XY:115:VAL:HG22	55:XY:203:VAL:HG22	1.87	0.56
1:RA:729:G:C8	3:RD:208:LYS:HD2	2.40	0.56
1:RA:2115:G:H21	1:RA:2171:A:H61	1.54	0.56
1:RA:2452:C:H4'	55:QY:239:THR:HG21	1.86	0.56
8:RI:92:VAL:HG13	8:RI:120:ILE:HB	1.87	0.56
13:RR:28:LEU:HD12	13:RR:44:LEU:HD13	1.86	0.56
32:QA:1013:G:N2	32:QA:1016:A:OP2	2.37	0.56
35:QD:168:ARG:HH21	3:YD:135:PHE:HE1	1.52	0.56
1:YA:566:U:H5''	11:YP:29:LYS:HE3	1.87	0.56
1:YA:1359:A:N6	1:YA:1372:U:H3	2.01	0.56
1:YA:1794:U:H2'	1:YA:1795:C:C6	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:YD:10:THR:OG1	3:YD:13:ARG:HG2	2.05	0.56
44:XM:19:LEU:HD21	44:XM:56:LEU:HD21	1.87	0.56
1:RA:1569:A:H5'	3:RD:61:LEU:HD11	1.86	0.56
6:RG:59:GLU:OE2	6:RG:153:ARG:NH2	2.38	0.56
6:RG:108:ASN:O	26:R4:37:SER:N	2.38	0.56
39:QH:10:LEU:HD22	39:QH:83:ILE:HD11	1.88	0.56
47:QP:75:ARG:HG3	47:QP:80:PHE:HD2	1.70	0.56
1:YA:749:C:O2	1:YA:1618:A:H2'	2.06	0.56
1:YA:1124:C:O2'	31:Y9:36:GLN:HG2	2.05	0.56
22:R0:11:ARG:O	22:R0:14:ARG:NH2	2.38	0.56
32:QA:194:C:H2'	32:QA:195:A:H5''	1.87	0.56
1:YA:2206:G:H5''	1:YA:2207:G:N7	2.21	0.56
1:YA:2243:U:H2'	1:YA:2244:U:C6	2.41	0.56
1:RA:530:G:N1	1:RA:2023:G:OP1	2.30	0.56
1:RA:2807:G:N1	1:RA:2893:G:O6	2.34	0.56
1:YA:740:U:H2'	1:YA:741:G:C8	2.41	0.56
34:XC:179:ARG:NH1	34:XC:206:GLU:OE1	2.38	0.56
40:XI:50:LEU:HB2	40:XI:56:LEU:HD23	1.87	0.56
1:RA:83:G:OP1	20:RY:95:LYS:NZ	2.30	0.56
1:RA:2115:G:N1	1:RA:2119:A:OP2	2.39	0.56
32:QA:109:A:C6	32:QA:326:G:C6	2.94	0.56
33:QB:229:VAL:HG12	33:QB:230:VAL:H	1.70	0.56
48:QQ:66:SER:O	48:QQ:70:ARG:NH1	2.39	0.56
1:YA:644:A:H4'	1:YA:645:C:H5	1.70	0.56
7:YH:89:ILE:O	7:YH:129:THR:HG23	2.06	0.56
14:YS:14:VAL:O	14:YS:18:ILE:HG12	2.06	0.56
15:YT:60:THR:HG22	15:YT:77:PRO:HA	1.88	0.56
55:XY:224:ILE:HD13	55:XY:267:LYS:HE3	1.86	0.56
1:RA:272(M):G:H21	8:RI:50:ARG:HD3	1.70	0.56
1:RA:539:G:H2'	1:RA:540:C:C6	2.40	0.56
1:RA:1065:U:H4'	1:RA:1066:U:H5'	1.87	0.56
1:RA:2698:U:H2'	1:RA:2699:C:C6	2.41	0.56
1:YA:184:C:H2'	1:YA:185:U:C6	2.40	0.56
1:YA:1143:A:OP1	9:YN:25:ARG:NH2	2.39	0.56
1:YA:1649:G:O2'	13:YR:107:ASP:OD2	2.16	0.56
1:YA:2785:C:O2'	4:YE:66:HIS:ND1	2.36	0.56
32:XA:35:G:O2'	43:XL:118:SER:O	2.21	0.56
35:XD:153:ARG:HH12	35:XD:181:MET:HB2	1.71	0.56
1:RA:2889:C:H3'	1:RA:2891:G:C8	2.41	0.56
7:RH:86:GLU:OE2	7:RH:132:ARG:NH2	2.39	0.56
1:YA:1050:A:H2'	1:YA:1051:G:H8	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:YA:1076:C:H4'	1:YA:1077:A:OP1	2.06	0.56
1:YA:2889:C:H3'	1:YA:2891:G:C8	2.40	0.56
23:Y1:3:LYS:HB2	23:Y1:61:ARG:NH1	2.21	0.56
8:RI:38:LEU:H	8:RI:38:LEU:HD12	1.71	0.56
32:QA:1427:U:H2'	32:QA:1428:A:C8	2.41	0.56
37:QF:89:MET:HE1	49:QR:72:ARG:HB3	1.88	0.56
10:YO:23:ARG:HD3	10:YO:24:VAL:N	2.21	0.56
39:XH:6:ILE:HB	39:XH:85:ARG:NH1	2.21	0.56
41:XJ:37:PRO:HA	41:XJ:72:VAL:HG12	1.86	0.56
1:RA:1062:G:N7	1:RA:1070:A:H1'	2.21	0.55
32:QA:1003:G:H2'	32:QA:1004:A:H4'	1.87	0.55
6:YG:46:ALA:HB2	6:YG:53:LEU:HG	1.87	0.55
32:XA:1075:C:OP1	33:XB:179:LYS:NZ	2.24	0.55
55:XY:110:ASN:OD1	55:XY:167:SER:HA	2.06	0.55
34:QC:155:GLY:HA3	34:QC:196:LEU:HD22	1.88	0.55
55:QY:312:PHE:N	55:QY:313:PRO:HD2	2.20	0.55
36:XE:10:MET:HB3	36:XE:13:ILE:HD11	1.88	0.55
55:XY:147:GLU:HB3	55:XY:165:LYS:HB3	1.88	0.55
1:RA:1057:A:N7	1:RA:1086:A:H2'	2.21	0.55
26:R4:59:PHE:HE1	50:QS:64:GLU:HA	1.71	0.55
32:QA:38:G:N2	32:QA:397:A:H5'	2.20	0.55
1:YA:588:U:H2'	1:YA:589:C:C6	2.41	0.55
1:YA:1308:A:H2'	1:YA:1309:G:O4'	2.06	0.55
1:YA:2355:C:H1'	22:Y0:39:ARG:HH21	1.71	0.55
43:XL:33:ARG:HD3	43:XL:62:SER:HB3	1.88	0.55
32:QA:406:G:H5'	35:QD:5:ILE:HD11	1.89	0.55
15:YT:54:ARG:HA	15:YT:59:THR:HG23	1.88	0.55
16:YU:76:TYR:OH	16:YU:92:ARG:NH1	2.39	0.55
1:RA:574:C:N3	4:RE:145:LYS:NZ	2.55	0.55
1:RA:1053:C:H2'	1:RA:1054:A:C8	2.42	0.55
1:RA:1935:G:H1'	1:RA:1964:G:N2	2.22	0.55
5:RF:185:ASP:HA	5:RF:188:ARG:HD3	1.88	0.55
34:QC:8:ILE:HD12	34:QC:16:ARG:HD3	1.88	0.55
38:QG:48:LYS:O	38:QG:52:GLU:HG2	2.06	0.55
55:QY:263:GLN:O	55:QY:267:LYS:N	2.40	0.55
55:QY:330:ASP:O	55:QY:334:GLU:HB3	2.05	0.55
1:YA:833:U:O2	11:YP:55:ARG:NH2	2.40	0.55
26:Y4:53:GLU:CD	26:Y4:53:GLU:H	2.09	0.55
1:RA:2094:G:P	8:RI:22:LYS:HD2	2.47	0.55
10:RO:2:ILE:HB	10:RO:33:ALA:HB3	1.88	0.55
1:RA:1292:U:H2'	1:RA:1293:C:C6	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:QD:3:ARG:HD3	35:QD:118:ARG:NE	2.14	0.55
6:YG:5:VAL:HG12	26:Y4:25:TYR:CE1	2.42	0.55
34:XC:6:HIS:CE1	34:XC:8:ILE:HB	2.42	0.55
1:RA:2816:C:O3'	13:RR:99:LYS:NZ	2.39	0.55
32:QA:1503:A:OP1	32:QA:1531:A:O2'	2.25	0.55
41:QJ:38:ILE:HD11	41:QJ:71:LEU:HD23	1.88	0.55
44:QM:40:ASN:HB3	44:QM:43:THR:HG23	1.89	0.55
10:YO:115:VAL:HG13	10:YO:121:VAL:HG21	1.89	0.55
43:XL:32:PHE:CD2	43:XL:86:ARG:HB3	2.41	0.55
44:XM:6:GLY:HA3	44:XM:67:GLU:HG3	1.89	0.55
46:XO:4:THR:HG23	46:XO:7:GLU:H	1.72	0.55
1:RA:1076:C:H4'	1:RA:1077:A:OP1	2.07	0.55
1:RA:2156:G:N7	1:RA:2157:G:N2	2.54	0.55
15:RT:39:ARG:NH1	15:RT:41:ARG:HD3	2.22	0.55
12:YQ:16:ARG:HG3	12:YQ:17:LEU:H	1.72	0.55
1:RA:299:A:N1	1:RA:322:A:O2'	2.31	0.55
1:RA:2171:A:H4'	1:RA:2172:U:OP1	2.07	0.55
1:RA:2648:C:H2'	1:RA:2649:U:C6	2.42	0.55
1:YA:192:C:O2'	1:YA:802:A:N3	2.31	0.55
1:YA:212:G:H2'	1:YA:213:A:O4'	2.07	0.55
1:YA:2646:C:OP2	1:YA:2732:G:O2'	2.18	0.55
24:Y2:35:LEU:HD12	24:Y2:53:LEU:HD12	1.89	0.55
33:XB:88:ALA:HB2	33:XB:219:VAL:HG13	1.89	0.55
40:XI:51:ARG:HG2	40:XI:56:LEU:HD21	1.89	0.55
1:RA:2023:G:H5'	1:RA:2617:C:H4'	1.89	0.54
1:RA:2683:C:OP1	15:RT:53:ARG:NH2	2.40	0.54
13:RR:36:THR:HG22	13:RR:37:THR:H	1.72	0.54
14:RS:14:VAL:O	14:RS:18:ILE:HG12	2.07	0.54
30:R8:52:LYS:O	30:R8:56:GLU:HG3	2.07	0.54
32:QA:1441:G:H5''	32:QA:1442(A):G:H5'	1.88	0.54
55:QY:135:TYR:HE1	55:QY:178:GLU:HG3	1.72	0.54
1:YA:458:G:O2'	1:YA:469:G:O6	2.18	0.54
1:YA:641:C:O2'	1:YA:2350:C:OP1	2.22	0.54
1:YA:1657:C:H2'	1:YA:1658:C:H6	1.71	0.54
32:XA:266:G:H3'	48:XQ:67:LYS:HB2	1.88	0.54
1:RA:372:G:H5'	23:R1:66:HIS:NE2	2.22	0.54
1:RA:589:C:H2'	1:RA:590:A:C8	2.42	0.54
1:RA:2206:G:H5''	1:RA:2207:G:C8	2.42	0.54
1:RA:2646:C:OP2	1:RA:2732:G:O2'	2.22	0.54
1:RA:2744:G:N2	7:RH:143:GLN:OE1	2.39	0.54
1:RA:2839:G:H5'	13:RR:46:GLY:HA2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:RT:24:PRO:HD3	15:RT:52:ILE:HD12	1.89	0.54
32:QA:1020:U:H2'	32:QA:1021:G:H8	1.72	0.54
33:QB:21:ARG:H	33:QB:21:ARG:HD3	1.70	0.54
35:QD:98:GLU:OE1	35:QD:103:ASN:ND2	2.38	0.54
39:QH:51:VAL:HG12	39:QH:52:ASP:H	1.72	0.54
1:YA:829:A:N7	1:YA:2247:A:O2'	2.39	0.54
55:XY:133:ARG:HG3	55:XY:134:MET:HE2	1.87	0.54
3:RD:183:ARG:HH11	3:RD:183:ARG:HG3	1.72	0.54
5:RF:184:TYR:CE2	5:RF:188:ARG:HD2	2.43	0.54
12:RQ:16:ARG:HG2	12:RQ:18:LYS:HG3	1.89	0.54
26:R4:16:CYS:SG	26:R4:17:GLY:N	2.80	0.54
40:QI:77:ILE:O	40:QI:81:ILE:HG23	2.07	0.54
1:YA:1796:U:H2'	1:YA:1797:C:C6	2.42	0.54
4:YE:24:THR:HG23	4:YE:186:GLY:O	2.05	0.54
32:XA:474:G:H2'	32:XA:475:G:C8	2.41	0.54
32:XA:1118:C:H1'	32:XA:1179:A:C4	2.42	0.54
42:XK:116:HIS:N	42:XK:117:ASN:HA	2.22	0.54
55:XY:127:PHE:HA	55:XY:130:ASP:HB2	1.89	0.54
1:RA:1530:C:H42	1:RA:1539:G:H1	1.54	0.54
27:R5:49:CYS:HA	27:R5:60:VAL:HG11	1.90	0.54
32:QA:341:C:H2'	32:QA:342:C:C6	2.43	0.54
37:QF:100:ASN:ND2	49:QR:26:LEU:O	2.40	0.54
40:QI:46:ALA:HB2	40:QI:74:ILE:HG23	1.89	0.54
1:YA:250:G:P	30:Y8:13:ARG:HH22	2.30	0.54
1:YA:1087:G:N2	1:YA:1102:C:N3	2.41	0.54
1:YA:1364:G:OP2	23:Y1:3:LYS:HG3	2.08	0.54
36:XE:33:VAL:HG21	36:XE:109:ILE:HA	1.89	0.54
55:XY:229:SER:HA	55:XY:258:GLN:OE1	2.08	0.54
1:RA:1011:G:H1'	1:RA:1013:C:O4'	2.06	0.54
1:RA:1073:A:H2'	1:RA:1074:G:H8	1.71	0.54
1:RA:1903:G:OP1	3:RD:241:PRO:HB2	2.07	0.54
3:RD:69:ARG:HG2	3:RD:69:ARG:NH1	2.21	0.54
32:QA:976:G:H5'	32:QA:1358:U:O2'	2.08	0.54
44:QM:80:ARG:O	44:QM:84:ILE:HG23	2.08	0.54
32:XA:1146:A:H3'	32:XA:1147:C:H5''	1.89	0.54
33:XB:178:ARG:NH2	39:XH:74:PRO:HB3	2.23	0.54
34:XC:150:LYS:HG3	34:XC:169:ALA:HB2	1.90	0.54
1:RA:2611:U:C4	27:R5:3:LYS:HG2	2.43	0.54
1:YA:1378:A:OP1	29:Y7:10:ARG:NH2	2.40	0.54
1:YA:1530:C:H42	1:YA:1539:G:H1	1.56	0.54
1:YA:2081:C:H2'	1:YA:2082:A:H8	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:YA:2206:G:H8	1:YA:2207:G:N7	2.05	0.54
1:YA:2336:A:H61	22:Y0:43:THR:CG2	2.21	0.54
7:YH:11:VAL:HG21	7:YH:50:VAL:HG23	1.90	0.54
32:XA:975:A:N1	41:XJ:48:THR:HB	2.23	0.54
35:XD:70:ILE:HD11	35:XD:74:GLN:HB3	1.90	0.54
1:RA:270:A:OP2	1:RA:272(X):G:N1	2.33	0.54
1:RA:2111:C:H42	1:RA:2147:G:H22	1.54	0.54
1:YA:1075:C:H2'	1:YA:1076:C:H5'	1.88	0.54
1:YA:2757:A:P	31:Y9:20:HIS:H	2.30	0.54
1:RA:1385:G:O2'	1:RA:1396:U:O2	2.25	0.54
1:YA:2031:A:C6	1:YA:2498:C:H1'	2.43	0.54
32:XA:1305:G:N2	32:XA:1331:G:H1'	2.23	0.54
32:XA:1391:U:H2'	32:XA:1392:G:C8	2.43	0.54
33:XB:16:HIS:CG	33:XB:210:SER:HB3	2.42	0.54
1:RA:607:U:OP1	5:RF:102:PRO:HA	2.08	0.54
11:RP:52:GLU:OE1	11:RP:55:ARG:NH1	2.40	0.54
13:RR:83:ILE:O	13:RR:86:ARG:HG2	2.08	0.54
19:RX:11:PRO:HB3	19:RX:92:LEU:HD11	1.88	0.54
32:QA:1414:U:H3	32:QA:1486:G:H1	1.56	0.54
1:YA:1117:G:H2'	1:YA:1118:C:C6	2.42	0.54
33:XB:84:GLU:HB3	33:XB:219:VAL:HG21	1.90	0.54
1:RA:2577:A:OP2	27:R5:3:LYS:NZ	2.29	0.54
32:QA:1492:A:H4'	43:QL:47:LYS:NZ	2.22	0.54
34:QC:6:HIS:CE1	34:QC:8:ILE:HB	2.43	0.54
1:YA:889:C:O2'	1:YA:890:A:O5'	2.24	0.54
1:YA:2345:G:N3	1:YA:2381:C:H2'	2.23	0.54
7:YH:46:GLU:HB2	7:YH:49:VAL:HG12	1.89	0.54
42:XK:115:PRO:C	42:XK:117:ASN:HA	2.27	0.54
1:RA:1686:C:H2'	1:RA:1687:G:O4'	2.07	0.53
1:RA:1847:A:H3'	1:RA:1848:A:H5'	1.90	0.53
4:RE:119:ARG:HD2	4:RE:120:TRP:CE2	2.43	0.53
6:RG:179:PRO:HB2	26:R4:42:PHE:CE2	2.37	0.53
7:RH:8:PRO:C	7:RH:69:ARG:HH12	2.11	0.53
33:QB:54:THR:HG21	33:QB:201:ILE:HD11	1.89	0.53
1:YA:634:C:H2'	1:YA:635:C:C6	2.43	0.53
1:YA:1084:A:H3'	1:YA:1085:A:H4'	1.88	0.53
1:YA:1432:C:H2'	1:YA:1433:U:O4'	2.08	0.53
4:YE:14:ILE:HG13	4:YE:21:VAL:HG13	1.90	0.53
30:Y8:23:VAL:HG11	30:Y8:47:LYS:HD3	1.89	0.53
32:XA:486:U:H2'	32:XA:487:A:C8	2.40	0.53
32:XA:501:C:H2'	32:XA:502:G:H8	1.71	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:XA:1286:A:H2'	32:XA:1287:A:H4'	1.90	0.53
1:RA:1028:A:N3	1:RA:2486:G:O2'	2.33	0.53
15:RT:53:ARG:HB3	15:RT:53:ARG:HH11	1.73	0.53
32:QA:1187:G:H4'	40:QI:111:ARG:HH11	1.72	0.53
6:YG:113:ARG:HD2	6:YG:140:ILE:O	2.08	0.53
7:YH:115:VAL:HG11	7:YH:148:ILE:HD11	1.90	0.53
32:XA:859:A:H2'	32:XA:860:A:O4'	2.09	0.53
38:XG:132:GLY:O	38:XG:136:LYS:HG2	2.07	0.53
46:XO:25:THR:HG21	46:XO:70:LEU:HB2	1.91	0.53
47:XP:19:ILE:HG22	47:XP:36:ILE:HG13	1.90	0.53
1:RA:1057:A:O2'	1:RA:1058:G:OP1	2.25	0.53
1:RA:2122:U:H3	1:RA:2176:A:H61	1.55	0.53
17:RV:72:VAL:HG13	17:RV:85:LYS:HB3	1.90	0.53
32:QA:1260:C:H4'	32:QA:1284:C:H5'	1.89	0.53
32:XA:148:G:H2'	32:XA:149:A:H8	1.73	0.53
40:XI:16:ARG:HH11	40:XI:64:THR:HG21	1.73	0.53
4:RE:143:ASN:HD22	4:RE:147:PRO:HD3	1.72	0.53
17:RV:76:LYS:HB2	17:RV:81:TYR:HB3	1.90	0.53
32:QA:1003:G:N2	32:QA:1004:A:H1'	2.24	0.53
55:QY:177:PHE:O	55:QY:321:ARG:NH2	2.41	0.53
1:YA:1064:C:H3'	1:YA:1065:U:C5'	2.38	0.53
5:YF:24:LEU:HD23	5:YF:115:ALA:HA	1.89	0.53
7:YH:154:PRO:HB3	7:YH:163:TYR:CE2	2.43	0.53
1:RA:642:G:N2	1:RA:645:C:OP2	2.41	0.53
1:RA:2031:A:N3	1:RA:2455:G:O2'	2.30	0.53
12:RQ:16:ARG:HG3	12:RQ:17:LEU:H	1.73	0.53
43:QL:71:PRO:O	43:QL:102:ARG:NH1	2.41	0.53
1:YA:309:G:N3	1:YA:329:G:O2'	2.38	0.53
1:YA:2119:A:H61	1:YA:2168:G:H21	1.56	0.53
32:XA:600:C:H2'	32:XA:601:C:C6	2.44	0.53
43:XL:28:LYS:N	43:XL:29:GLY:HA2	2.24	0.53
5:RF:197:ASP:N	5:RF:197:ASP:OD1	2.42	0.53
35:QD:61:LYS:NZ	35:QD:72:GLU:OE2	2.41	0.53
1:YA:1062:G:N7	1:YA:1070:A:H1'	2.24	0.53
1:YA:1184:G:OP1	25:Y3:30:ARG:HD2	2.08	0.53
1:YA:2144:U:O2'	1:YA:2147:G:N1	2.40	0.53
32:XA:359:U:H2'	32:XA:360:A:H8	1.73	0.53
1:YA:2171:A:H4'	1:YA:2172:U:OP1	2.07	0.53
1:YA:2698:U:H2'	1:YA:2699:C:C6	2.44	0.53
32:XA:437:U:H5'	35:XD:155:LEU:HD21	1.90	0.53
35:XD:173:TRP:CD1	35:XD:174:LEU:HG	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:RA:1049:C:H42	1:RA:2751:G:H1	1.56	0.53
1:RA:1268:A:H2'	1:RA:1269:A:O4'	2.08	0.53
1:RA:1971:A:C4	3:RD:241:PRO:HD3	2.44	0.53
1:RA:2074:U:H2'	1:RA:2075:U:C6	2.44	0.53
3:RD:71:ASP:HB3	3:RD:103:ARG:NH2	2.22	0.53
32:QA:1034:G:H3'	32:QA:1035:A:C8	2.43	0.53
32:QA:1516:G:N1	32:QA:1519:MA6:OP2	2.41	0.53
33:QB:69:LEU:HB3	33:QB:162:ILE:HG22	1.91	0.53
41:QJ:37:PRO:HA	41:QJ:72:VAL:HG12	1.90	0.53
1:YA:1296:G:OP1	1:YA:2709:G:O2'	2.20	0.53
1:YA:1514:U:H2'	1:YA:1515:G:C8	2.43	0.53
15:YT:24:PRO:HD3	15:YT:52:ILE:HD12	1.91	0.53
38:XG:27:ILE:HD12	38:XG:40:ALA:HA	1.89	0.53
49:XR:31:LEU:HD21	49:XR:62:GLU:HB2	1.91	0.53
1:RA:1769:G:O2'	1:RA:1958:C:OP1	2.19	0.53
1:YA:1416:G:O2'	1:YA:1417:C:OP2	2.23	0.53
1:YA:2336:A:H61	22:Y0:43:THR:HG22	1.74	0.53
7:YH:137:ASP:HB3	7:YH:140:LYS:HB3	1.91	0.53
21:YZ:125:LEU:HB3	21:YZ:165:VAL:HG13	1.91	0.53
32:XA:142:G:H2'	32:XA:143:A:H8	1.74	0.53
32:XA:1347:G:N2	32:XA:1373:G:H2'	2.24	0.53
1:RA:11:G:H2'	1:RA:12:U:H5'	1.91	0.53
1:RA:876:C:H2'	1:RA:877:U:O4'	2.10	0.53
16:RU:108:GLU:HG2	17:RV:45:THR:HG21	1.90	0.53
32:QA:581:G:OP1	46:QO:61:GLY:HA3	2.09	0.53
32:QA:1492:A:H8	55:QY:119:THR:HG21	1.74	0.53
55:QY:257:CYS:O	55:QY:266:ASN:ND2	2.35	0.53
1:YA:78:A:H2'	1:YA:79:G:C8	2.43	0.53
6:YG:55:LYS:HA	6:YG:58:GLN:HB3	1.90	0.53
37:XF:37:VAL:HA	37:XF:65:VAL:HG12	1.91	0.53
43:XL:83:VAL:HG13	43:XL:100:ILE:HG23	1.91	0.53
1:RA:362:U:O2'	1:RA:363(A):G:H5'	2.09	0.52
1:RA:1991:U:H2'	1:RA:1992:G:H5''	1.92	0.52
32:QA:159:G:N2	32:QA:161:A:H3'	2.24	0.52
32:QA:921:U:O2'	36:QE:19:MET:O	2.18	0.52
38:QG:45:ASP:O	38:QG:49:ILE:HG13	2.08	0.52
54:QX:21:A:H62	55:QY:198:THR:HG1	1.54	0.52
1:YA:2189:U:H2'	1:YA:2190:G:C8	2.44	0.52
17:YV:29:PRO:HA	17:YV:61:VAL:HG23	1.89	0.52
21:YZ:33:LEU:HD11	21:YZ:90:VAL:HG21	1.90	0.52
32:XA:769:G:H4'	32:XA:1513:A:H4'	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:XD:173:TRP:CD1	35:XD:189:PRO:HG3	2.44	0.52
43:XL:70:ILE:HG12	43:XL:100:ILE:HD12	1.90	0.52
1:RA:247:G:H4'	1:RA:386:G:C5	2.44	0.52
1:RA:2232:U:OP1	23:R1:40:ARG:NH1	2.39	0.52
6:RG:50:ALA:C	6:RG:52:ILE:H	2.13	0.52
32:QA:17:U:H2'	32:QA:18:C:C6	2.44	0.52
32:QA:188:C:O4'	51:QT:89:ARG:NH2	2.42	0.52
10:YO:80:ASP:OD1	15:YT:64:ARG:NH2	2.42	0.52
32:XA:1004:A:H5'	32:XA:1025:U:H5	1.73	0.52
35:XD:79:PHE:HE1	35:XD:204:ILE:HD13	1.74	0.52
40:XI:9:ARG:HG2	40:XI:14:VAL:HG12	1.91	0.52
4:RE:105:THR:OG1	4:RE:199:ARG:NH2	2.43	0.52
38:QG:150:ALA:HA	42:QK:59:TYR:HB3	1.92	0.52
41:QJ:11:PHE:HE1	41:QJ:67:THR:HG22	1.74	0.52
5:YF:178:PRO:HB2	5:YF:201:VAL:CG2	2.37	0.52
8:YI:14:ASP:OD1	8:YI:15:VAL:N	2.41	0.52
12:YQ:30:GLY:HA2	12:YQ:107:ALA:HB2	1.89	0.52
40:XI:53:VAL:C	40:XI:55:ALA:H	2.11	0.52
47:XP:23:ASP:OD1	47:XP:25:ARG:HD3	2.10	0.52
55:XY:212:ALA:CB	55:XY:214:LEU:HG	2.37	0.52
55:XY:312:PHE:N	55:XY:313:PRO:HD2	2.24	0.52
1:RA:1101:U:H2'	1:RA:1102:C:H6	1.75	0.52
1:RA:1139:G:O2'	1:RA:1143:A:N1	2.31	0.52
1:RA:1756:G:H4'	1:RA:1758:G:O4'	2.10	0.52
9:RN:120:LEU:HD22	9:RN:122:VAL:HG23	1.91	0.52
32:QA:539:A:OP2	43:QL:115:LYS:NZ	2.43	0.52
38:QG:79:ARG:HA	38:QG:84:ASN:HA	1.91	0.52
1:YA:2438:U:O2'	1:YA:2440:C:OP1	2.23	0.52
24:Y2:17:SER:OG	24:Y2:20:GLU:HG3	2.09	0.52
32:XA:1117:G:H4'	40:XI:104:ARG:NH1	2.24	0.52
1:RA:1068:G:H3'	1:RA:1096:A:OP2	2.10	0.52
1:RA:1081:U:H3'	1:RA:1085:A:H61	1.74	0.52
1:RA:2567:G:H2'	1:RA:2568:C:C6	2.45	0.52
7:RH:59:ARG:HH11	7:RH:59:ARG:HG2	1.75	0.52
32:QA:1292:U:OP2	38:QG:41:ARG:NH2	2.43	0.52
36:QE:102:ALA:HB1	36:QE:106:PRO:HG2	1.91	0.52
44:QM:34:LEU:HD13	44:QM:41:PRO:HA	1.90	0.52
55:QY:98:VAL:C	55:QY:100:LEU:H	2.13	0.52
1:YA:277:C:O2'	1:YA:278:A:OP1	2.19	0.52
1:YA:1057:A:N7	1:YA:1086:A:H2'	2.24	0.52
1:YA:1239:G:H2'	1:YA:1240:U:O4'	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:YA:1530:C:HO2'	1:YA:1531:C:P	2.30	0.52
1:YA:2128:C:N4	1:YA:2160:G:H1	2.04	0.52
1:RA:2032:G:H1'	4:RE:145:LYS:HD3	1.92	0.52
1:RA:2110:G:H5''	1:RA:2111:C:H5	1.75	0.52
32:QA:1004:A:O2'	32:QA:1038:C:O2	2.16	0.52
33:QB:16:HIS:HB3	33:QB:210:SER:HB2	1.92	0.52
44:QM:13:LYS:HA	44:QM:44:ARG:HH11	1.73	0.52
1:YA:1102:C:H2'	1:YA:1103:A:C8	2.45	0.52
6:YG:11:TYR:CZ	6:YG:16:ARG:HD2	2.45	0.52
20:YY:23:ARG:HG3	20:YY:42:VAL:HG22	1.92	0.52
1:RA:2130:U:H2'	1:RA:2158:A:H61	1.75	0.52
32:QA:519:C:OP1	55:QY:183:ARG:NH1	2.43	0.52
35:QD:116:GLN:NE2	35:QD:157:LEU:HD11	2.24	0.52
48:QQ:67:LYS:HA	48:QQ:70:ARG:HH12	1.74	0.52
1:YA:644:A:H4'	1:YA:645:C:C5	2.44	0.52
1:YA:1068:G:H3'	1:YA:1096:A:OP2	2.10	0.52
1:YA:2065:C:H2'	1:YA:2066:C:C6	2.45	0.52
1:YA:2334:G:H5'	14:YS:9:ARG:HG2	1.91	0.52
5:YF:165:ARG:HG2	5:YF:168:ARG:NH2	2.25	0.52
1:RA:922:U:H2'	1:RA:923:C:C6	2.45	0.52
1:RA:1259:G:H2'	1:RA:1260:G:C8	2.45	0.52
44:QM:76:ALA:HA	44:QM:79:LYS:HB3	1.91	0.52
1:YA:336:C:O2'	20:YY:35:TYR:OH	2.23	0.52
28:Y6:6:ARG:NE	28:Y6:24:GLU:OE1	2.35	0.52
32:XA:123:C:OP1	32:XA:311:C:O2'	2.25	0.52
32:XA:660:G:H1	32:XA:745:C:H42	1.58	0.52
39:XH:51:VAL:HG11	39:XH:60:ARG:HH11	1.75	0.52
42:XK:82:VAL:HB	42:XK:108:ILE:HG12	1.91	0.52
44:XM:20:THR:HG21	44:XM:27:LYS:HD2	1.90	0.52
44:XM:81:LEU:HD13	44:XM:88:ARG:HD2	1.92	0.52
1:RA:2119:A:H61	1:RA:2168:G:H21	1.58	0.52
1:RA:2390:U:OP2	30:R8:35:GLN:NE2	2.34	0.52
8:RI:130:TYR:CE2	8:RI:132:PRO:HB3	2.45	0.52
11:RP:50:ARG:HD3	30:R8:7:HIS:CD2	2.45	0.52
1:YA:2127:G:H2'	1:YA:2128:C:O4'	2.09	0.52
12:YQ:32:TYR:OH	12:YQ:111:GLU:OE1	2.24	0.52
23:Y1:54:ALA:HB1	23:Y1:83:GLU:HG3	1.92	0.52
32:XA:1223:C:P	50:XS:78:ARG:HH22	2.32	0.52
33:XB:115:LEU:O	33:XB:119:GLU:HG2	2.10	0.52
36:XE:12:LEU:HD12	36:XE:128:PRO:HB2	1.92	0.52
1:RA:2018:G:O2'	16:RU:34:LYS:HE3	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:RA:2152:G:H2'	1:RA:2153:G:C8	2.44	0.52
1:RA:2165:G:H2'	1:RA:2166:G:O4'	2.10	0.52
2:RB:89:G:OP2	2:RB:89:G:H8	1.93	0.52
10:RO:97:ARG:NH1	32:QA:339:C:OP2	2.43	0.52
20:RY:90:LEU:HD21	20:RY:96:ILE:HG12	1.90	0.52
23:R1:51:VAL:HG11	23:R1:74:VAL:HG21	1.92	0.52
39:QH:6:ILE:O	39:QH:10:LEU:HG	2.10	0.52
1:YA:1514:U:H2'	1:YA:1515:G:H8	1.75	0.52
1:YA:2065:C:H2'	1:YA:2066:C:H6	1.75	0.52
1:YA:2111:C:H42	1:YA:2147:G:H22	1.57	0.52
1:YA:2280:G:O2'	1:YA:2388:A:N1	2.35	0.52
28:Y6:13:CYS:SG	28:Y6:47:THR:HG21	2.49	0.52
32:XA:390:C:H2'	32:XA:391:G:C8	2.45	0.52
35:XD:162:LEU:HD13	35:XD:181:MET:HG2	1.92	0.52
40:XI:4:TYR:HB2	40:XI:19:LEU:HB2	1.92	0.52
5:RF:20:LEU:HD23	5:RF:21:ALA:H	1.75	0.51
32:QA:337:C:H2'	32:QA:338:A:C8	2.45	0.51
32:QA:1086:U:H3	32:QA:1099:G:H22	1.58	0.51
40:QI:16:ARG:HD3	40:QI:64:THR:HG21	1.92	0.51
55:QY:221:ASP:HB3	55:QY:250:PRO:HD3	1.91	0.51
55:QY:338:ASP:N	55:QY:338:ASP:OD1	2.44	0.51
1:YA:455:C:N3	1:YA:472:A:H2'	2.25	0.51
1:YA:483:A:H5''	20:YY:50:ARG:HD3	1.92	0.51
32:XA:438:G:O2'	32:XA:494:U:O4	2.24	0.51
32:XA:1127:G:H5'	32:XA:1280:A:O2'	2.10	0.51
32:XA:1201:A:H4'	32:XA:1202:G:H5''	1.92	0.51
32:QA:1279:A:H5''	41:QJ:7:LYS:NZ	2.26	0.51
33:QB:73:THR:OG1	33:QB:170:GLU:OE1	2.27	0.51
34:QC:47:LEU:HD13	34:QC:68:VAL:HG11	1.92	0.51
35:QD:76:ARG:HD3	35:QD:207:TYR:CE1	2.45	0.51
55:QY:115:VAL:HG22	55:QY:203:VAL:HG22	1.92	0.51
17:YV:35:LEU:HB2	17:YV:57:VAL:HG22	1.93	0.51
19:YX:57:LEU:HD11	19:YX:78:LYS:HE3	1.92	0.51
32:XA:1015:A:H2'	32:XA:1016:A:C8	2.45	0.51
1:RA:1739:U:HO2'	1:RA:1740:G:H8	1.58	0.51
21:RZ:92:SER:O	21:RZ:130:PRO:HG2	2.11	0.51
32:QA:833:U:H2'	32:QA:834:C:H6	1.74	0.51
35:QD:170:VAL:HG12	35:QD:174:LEU:HB2	1.91	0.51
37:QF:69:GLU:O	37:QF:72:VAL:HG12	2.10	0.51
1:YA:322:A:OP1	5:YF:168:ARG:HD2	2.11	0.51
1:YA:952:G:P	12:YQ:16:ARG:HH22	2.33	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:YA:1067:A:H4'	1:YA:1068:G:OP2	2.09	0.51
21:YZ:19:ARG:NH1	21:YZ:84:GLU:O	2.44	0.51
32:XA:1002:G:H2'	32:XA:1003:G:C8	2.45	0.51
55:XY:342:GLU:O	55:XY:346:GLN:N	2.36	0.51
1:RA:272(E):U:H2'	1:RA:272(F):C:C6	2.45	0.51
1:RA:2128:C:N4	1:RA:2160:G:H1	2.06	0.51
6:RG:9:ARG:O	6:RG:13:GLU:HG3	2.09	0.51
32:QA:614:A:OP1	35:QD:85:LYS:NZ	2.43	0.51
1:YA:811:U:H2'	11:YP:21:ARG:HA	1.91	0.51
1:YA:958:U:O2'	1:YA:959:A:OP2	2.24	0.51
4:YE:111:ARG:HG2	4:YE:160:TYR:O	2.11	0.51
32:XA:767:A:H2'	32:XA:768:A:O4'	2.09	0.51
32:XA:1158:C:O2	32:XA:1158:C:H2'	2.09	0.51
33:XB:179:LYS:HG2	39:XH:72:PRO:HG3	1.92	0.51
35:XD:8:VAL:HG22	35:XD:21:LEU:HD13	1.92	0.51
39:XH:41:ARG:NH2	39:XH:123:GLU:OE2	2.43	0.51
51:XT:37:SER:O	51:XT:41:ILE:HG12	2.10	0.51
1:RA:581:C:H2'	1:RA:582:G:C8	2.45	0.51
1:RA:944:G:H5''	1:RA:945:A:O5'	2.11	0.51
1:RA:2321:G:O2'	1:RA:2322:A:OP1	2.23	0.51
4:RE:36:ARG:HG2	4:RE:47:VAL:HG22	1.92	0.51
32:QA:102:G:O2'	32:QA:151:A:N3	2.36	0.51
1:YA:1866:C:H2'	1:YA:1876:A:O4'	2.10	0.51
1:YA:2033:A:O2'	1:YA:2035:G:OP2	2.24	0.51
1:YA:2430:A:H2'	1:YA:2430:A:N3	2.25	0.51
5:YF:21:ALA:HB3	5:YF:22:ALA:HA	1.91	0.51
32:XA:407:G:O2'	35:XD:116:GLN:HG3	2.10	0.51
35:XD:111:ALA:HB2	35:XD:120:LEU:HD12	1.92	0.51
55:XY:138:TYR:HD2	55:XY:337:LEU:H	1.59	0.51
1:RA:582:G:H2'	1:RA:583:G:H8	1.75	0.51
1:RA:1530:C:HO2'	1:RA:1531:C:P	2.34	0.51
1:RA:1791:A:N6	1:RA:1828:G:O2'	2.43	0.51
1:RA:2140:C:H2'	1:RA:2141:G:C8	2.37	0.51
11:RP:113:LYS:HA	11:RP:129:ALA:O	2.11	0.51
32:QA:537:G:H5''	43:QL:113:ARG:NH1	2.26	0.51
32:QA:769:G:H4'	32:QA:1513:A:H4'	1.91	0.51
32:QA:1216:G:H5''	45:QN:5:ALA:HB2	1.91	0.51
3:YD:16:MET:HG3	3:YD:206:LEU:O	2.11	0.51
46:XO:39:LEU:HD13	46:XO:56:LEU:HB2	1.92	0.51
1:RA:851:U:O2'	25:R3:42:ALA:O	2.29	0.51
1:RA:1086:A:OP1	1:RA:1104:C:O2'	2.29	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:RA:1187:G:H5'	17:RV:81:TYR:CE1	2.46	0.51
6:RG:62:LEU:O	6:RG:143:GLU:HG2	2.11	0.51
32:QA:410:G:OP1	35:QD:30:LYS:NZ	2.29	0.51
32:QA:1278:U:H5'	32:QA:1279:A:O4'	2.10	0.51
55:QY:332:VAL:HG22	55:QY:337:LEU:HB3	1.92	0.51
1:YA:1032:A:OP1	31:Y9:8:LYS:HE3	2.11	0.51
1:YA:1108:U:H3'	1:YA:1109:C:C6	2.45	0.51
24:Y2:16:LEU:O	24:Y2:67:LYS:NZ	2.44	0.51
47:XP:1:MET:SD	47:XP:65:GLN:HG3	2.51	0.51
1:RA:861:A:N3	2:RB:79:C:O2'	2.39	0.51
32:QA:67:C:H2'	32:QA:68:G:C8	2.46	0.51
55:QY:342:GLU:O	55:QY:346:GLN:N	2.37	0.51
1:YA:729:G:C8	3:YD:208:LYS:HD2	2.46	0.51
1:YA:2183:C:H2'	1:YA:2184:G:C8	2.45	0.51
32:XA:736:C:H2'	32:XA:737:A:C8	2.46	0.51
33:XB:124:SER:HB2	33:XB:125:PRO:HD3	1.91	0.51
38:XG:26:PHE:O	38:XG:30:ILE:HG13	2.11	0.51
55:XY:133:ARG:NH2	55:XY:334:GLU:OE1	2.44	0.51
55:XY:202:THR:HB	55:XY:298:LEU:HD22	1.93	0.51
1:RA:9:U:O2'	1:RA:10:G:OP1	2.26	0.51
1:RA:263:C:H2'	1:RA:264:C:O4'	2.11	0.51
1:RA:1593:G:H2'	1:RA:1594:G:C8	2.46	0.51
9:RN:15:LEU:HB2	9:RN:135:PRO:HB2	1.93	0.51
32:QA:1079:G:O3'	36:QE:14:ARG:NH2	2.44	0.51
33:QB:109:SER:O	33:QB:112:VAL:HG22	2.11	0.51
33:QB:231:GLU:HB3	33:QB:232:PRO:CD	2.35	0.51
49:XR:59:SER:OG	49:XR:62:GLU:HG2	2.11	0.51
1:RA:276:A:H5''	1:RA:277:C:H5'	1.92	0.51
1:RA:2689:U:OP2	1:RA:2719:G:N2	2.40	0.51
6:RG:116:ASP:OD1	44:QM:68:GLY:HA3	2.11	0.51
9:RN:67:LEU:O	9:RN:88:GLU:HG3	2.11	0.51
10:RO:23:ARG:HD3	10:RO:24:VAL:N	2.25	0.51
14:RS:25:ARG:HD3	14:RS:42:ASP:OD2	2.10	0.51
1:YA:1057:A:HO2'	1:YA:1058:G:P	2.34	0.51
1:YA:2627:G:O2'	1:YA:2781:A:N1	2.38	0.51
10:YO:64:ARG:HB2	10:YO:83:ALA:HB3	1.93	0.51
1:RA:873:G:H1	1:RA:904:C:H42	1.57	0.50
1:RA:1108:U:H3'	1:RA:1109:C:C6	2.46	0.50
6:RG:55:LYS:O	6:RG:59:GLU:HG3	2.11	0.50
32:QA:262:A:H2'	32:QA:263:A:C8	2.46	0.50
32:QA:1103:C:H2'	32:QA:1104:G:O4'	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:QA:1442(A):G:H1'	32:QA:1442(B):G:OP1	2.12	0.50
3:YD:142:VAL:HG23	3:YD:193:VAL:HA	1.92	0.50
13:YR:87:TYR:OH	13:YR:117:VAL:O	2.20	0.50
32:XA:396:G:O2'	32:XA:398:C:OP1	2.20	0.50
46:XO:7:GLU:OE2	46:XO:38:ARG:NH2	2.44	0.50
1:RA:583:G:OP2	16:RU:10:ARG:HD2	2.12	0.50
3:RD:242:ARG:H	3:RD:242:ARG:HD3	1.76	0.50
1:YA:276:A:H5''	1:YA:277:C:H4'	1.93	0.50
1:YA:764:A:H5'	3:YD:210:GLY:HA2	1.94	0.50
1:YA:1385:G:O2'	1:YA:1396:U:O2	2.25	0.50
1:YA:1693:U:O2'	3:YD:14:ARG:NH2	2.44	0.50
1:YA:2820:A:O2'	1:YA:2821:A:OP1	2.29	0.50
3:YD:183:ARG:HH11	3:YD:183:ARG:HG3	1.75	0.50
32:XA:1512:U:H2'	32:XA:1513:A:C8	2.46	0.50
35:XD:61:LYS:HD2	35:XD:207:TYR:OH	2.11	0.50
11:RP:8:PRO:HB2	11:RP:12:ALA:HB3	1.94	0.50
13:RR:56:LYS:NZ	13:RR:90:ARG:O	2.43	0.50
29:R7:30:VAL:O	29:R7:34:ARG:HG3	2.11	0.50
32:QA:73:G:H1	32:QA:96:U:H3	1.57	0.50
32:QA:1074:G:O2'	32:QA:1101:A:N1	2.39	0.50
32:QA:1124:G:N2	32:QA:1125:U:O4	2.45	0.50
1:YA:686:G:N2	1:YA:788:A:H61	2.09	0.50
1:YA:1639:U:C2'	1:YA:1640:C:H5''	2.40	0.50
1:YA:2074:U:H2'	1:YA:2075:U:C6	2.46	0.50
1:YA:2168:G:H22	1:YA:2171:A:H2'	1.75	0.50
1:YA:2572:A:C4	4:YE:144:ARG:NH1	2.79	0.50
6:YG:16:ARG:O	6:YG:20:ILE:HG13	2.12	0.50
32:XA:576:G:O6	32:XA:880:C:O2'	2.27	0.50
32:XA:748:C:H4'	32:XA:749:C:O5'	2.10	0.50
1:RA:1035:U:O5'	7:RH:59:ARG:NH1	2.44	0.50
1:RA:1278:A:OP1	13:RR:36:THR:HG23	2.11	0.50
6:RG:50:ALA:O	6:RG:52:ILE:N	2.45	0.50
9:RN:15:LEU:HD12	9:RN:137:LYS:HD3	1.92	0.50
32:QA:1343:G:H4'	40:QI:122:ALA:HB3	1.94	0.50
34:QC:70:VAL:HG22	34:QC:72:LYS:H	1.76	0.50
1:YA:384:U:H2'	1:YA:385:C:H6	1.76	0.50
1:YA:727:A:C6	1:YA:728:G:C6	3.00	0.50
1:YA:746:A:H2'	1:YA:2612:C:H5''	1.92	0.50
1:YA:2317:C:H2'	1:YA:2318:G:H5'	1.93	0.50
6:YG:3:LEU:H	6:YG:3:LEU:HD23	1.76	0.50
15:YT:108:ARG:NH1	32:XA:1464:G:OP1	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:XA:36:C:H5''	43:XL:123:LYS:HD3	1.92	0.50
32:XA:1327:C:H2'	32:XA:1328:C:C6	2.47	0.50
40:XI:21:PRO:HA	40:XI:59:PHE:HA	1.92	0.50
1:RA:900:A:H2'	1:RA:901:A:O4'	2.11	0.50
1:RA:1094:U:OP1	1:RA:1096:A:N6	2.45	0.50
10:RO:115:VAL:HG13	10:RO:121:VAL:HG21	1.93	0.50
19:RX:29:TRP:CE3	19:RX:78:LYS:HB3	2.47	0.50
19:RX:35:THR:HG22	19:RX:37:THR:H	1.76	0.50
1:YA:453:C:O2	1:YA:457:A:O2'	2.29	0.50
14:YS:25:ARG:HD3	14:YS:42:ASP:OD2	2.12	0.50
32:XA:719:C:O2'	49:XR:49:LYS:HB3	2.11	0.50
32:XA:1005:A:H5''	32:XA:1006:C:C5	2.47	0.50
32:XA:1015:A:N3	32:XA:1218:C:O2'	2.43	0.50
1:RA:729:G:C6	3:RD:208:LYS:HB2	2.47	0.50
1:RA:740:U:H2'	1:RA:741:G:C8	2.47	0.50
1:RA:2820:A:P	13:RR:2:ARG:HH22	2.35	0.50
3:RD:17:THR:O	3:RD:211:ARG:NH2	2.44	0.50
32:QA:328:C:H4'	32:QA:329:A:H5'	1.94	0.50
32:QA:1002:G:C6	32:QA:1003:G:C2	2.99	0.50
51:QT:89:ARG:O	51:QT:93:GLU:HG2	2.11	0.50
55:QY:255:VAL:HG12	55:QY:274:LEU:HG	1.93	0.50
1:YA:438:G:H2'	1:YA:440:G:H8	1.77	0.50
1:YA:1341:U:OP1	1:YA:1397:U:N3	2.40	0.50
1:YA:2115:G:N1	1:YA:2117:A:N7	2.59	0.50
1:YA:2267:A:H5''	1:YA:2268:A:H5'	1.93	0.50
6:YG:114:ILE:HG23	6:YG:136:ARG:NH2	2.27	0.50
11:YP:52:GLU:OE1	11:YP:55:ARG:NH1	2.43	0.50
32:XA:411:A:OP2	35:XD:25:ARG:NH2	2.44	0.50
33:XB:71:VAL:HG23	33:XB:164:VAL:HA	1.94	0.50
51:XT:18:GLN:O	51:XT:22:ARG:HG3	2.11	0.50
52:XU:5:ASP:O	52:XU:11:GLY:HA3	2.11	0.50
1:RA:848:G:H2'	1:RA:849:A:C8	2.47	0.50
1:RA:1224:C:O2'	17:RV:85:LYS:HA	2.11	0.50
1:RA:1750:G:O2'	1:RA:2860:A:N1	2.41	0.50
1:RA:2820:A:O2'	1:RA:2821:A:OP1	2.29	0.50
7:RH:20:ALA:HB3	7:RH:23:ARG:HG2	1.93	0.50
11:RP:60:MET:SD	30:R8:13:ARG:NH2	2.84	0.50
25:R3:3:ARG:NH1	25:R3:60:GLU:OE2	2.42	0.50
26:R4:51:ASP:CB	44:QM:65:LYS:HD2	2.41	0.50
28:R6:13:CYS:SG	28:R6:47:THR:HG21	2.51	0.50
32:QA:56:U:H2'	32:QA:57:G:C8	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:QD:172:PRO:HB2	35:QD:187:ARG:HH21	1.76	0.50
46:QO:29:VAL:HG11	46:QO:67:LEU:HD21	1.94	0.50
54:QX:21:A:N6	55:QY:198:THR:OG1	2.36	0.50
1:YA:2134:A:H8	1:YA:2156:G:H21	1.60	0.50
1:YA:2152:G:H2'	1:YA:2153:G:C8	2.47	0.50
1:YA:2839:G:H5'	13:YR:46:GLY:HA2	1.94	0.50
8:YI:130:TYR:HB3	8:YI:138:ILE:HB	1.94	0.50
50:XS:12:ASP:OD2	50:XS:35:SER:HB3	2.11	0.50
1:RA:26:G:H1'	1:RA:515:A:N6	2.27	0.50
1:RA:517:C:OP1	27:R5:16:ARG:NH2	2.45	0.50
1:RA:581:C:H2'	1:RA:582:G:H8	1.75	0.50
1:RA:2327:A:H2'	1:RA:2328:A:C8	2.46	0.50
5:RF:18:ARG:HG2	5:RF:19:GLU:N	2.26	0.50
7:RH:3:ARG:HB3	7:RH:6:ARG:HG2	1.94	0.50
36:QE:78:HIS:ND1	39:QH:104:ARG:HD2	2.26	0.50
55:QY:182:HIS:HB3	55:QY:310:TYR:HE2	1.77	0.50
1:YA:1608:A:H1'	1:YA:1610:A:OP2	2.12	0.50
1:YA:2114:A:H3'	1:YA:2115:G:H8	1.77	0.50
20:YY:102:CYS:SG	20:YY:104:GLY:N	2.75	0.50
30:Y8:6:THR:HG23	30:Y8:64:TYR:HD2	1.77	0.50
32:XA:600:C:H2'	32:XA:601:C:H6	1.76	0.50
32:XA:673:G:H2'	32:XA:674:G:C8	2.47	0.50
1:RA:1023:U:OP2	1:RA:1025:G:O2'	2.29	0.50
1:RA:1101:U:H2'	1:RA:1102:C:C6	2.46	0.50
1:RA:2189:U:H2'	1:RA:2190:G:C8	2.46	0.50
4:RE:12:THR:HG22	15:RT:58:ASN:HD21	1.77	0.50
51:QT:43:LEU:HD13	51:QT:51:GLU:HB3	1.93	0.50
1:YA:1301:A:C8	1:YA:1303:G:C8	3.00	0.50
1:YA:2304:G:H22	1:YA:2312:U:H3	1.58	0.50
1:YA:2636:U:OP1	4:YE:80:GLU:HB2	2.11	0.50
32:XA:662:G:H2'	32:XA:663:A:H8	1.76	0.50
32:XA:1002:G:N3	32:XA:1003:G:H8	2.10	0.50
32:XA:1129:C:N4	32:XA:1143:G:H1	2.09	0.50
40:XI:24:GLY:HA2	40:XI:59:PHE:O	2.12	0.50
44:XM:34:LEU:HD13	44:XM:41:PRO:HA	1.93	0.50
1:RA:479:A:N3	1:RA:481:G:H5''	2.27	0.49
5:RF:103:LYS:HA	5:RF:106:ARG:HD3	1.93	0.49
26:R4:54:GLY:O	26:R4:56:VAL:HA	2.12	0.49
32:QA:78:G:N2	32:QA:91:C:N3	2.55	0.49
32:QA:839:U:H1'	32:QA:840:C:OP1	2.12	0.49
39:QH:51:VAL:HG11	39:QH:60:ARG:HH12	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:QP:74:LEU:HD23	47:QP:79:VAL:HG21	1.93	0.49
1:YA:858:U:O2	1:YA:2268:A:H2'	2.12	0.49
1:YA:881:G:H2'	1:YA:882:G:C8	2.47	0.49
1:YA:2140:C:H2'	1:YA:2141:G:C8	2.41	0.49
32:XA:222:U:H2'	32:XA:223:U:C6	2.47	0.49
32:XA:343:U:H2'	32:XA:345:C:C5	2.47	0.49
32:QA:833:U:H2'	32:QA:834:C:C6	2.47	0.49
33:QB:8:LYS:HZ1	33:QB:52:GLU:HG3	1.76	0.49
35:QD:85:LYS:HD3	35:QD:86:LYS:N	2.27	0.49
49:QR:31:LEU:HD21	49:QR:62:GLU:HB3	1.93	0.49
53:QV:1:C:H42	53:QV:72:A:H61	1.60	0.49
5:YF:132:VAL:HA	5:YF:138:GLU:HB3	1.94	0.49
7:YH:9:ILE:O	7:YH:49:VAL:HA	2.12	0.49
12:YQ:38:GLU:HG3	12:YQ:127:ILE:HB	1.94	0.49
32:XA:524:G:H2'	32:XA:525:C:C6	2.47	0.49
32:XA:1040:U:H2'	32:XA:1041:A:O4'	2.12	0.49
33:XB:127:ILE:HG12	33:XB:128:GLU:H	1.76	0.49
51:XT:89:ARG:O	51:XT:93:GLU:HG2	2.12	0.49
55:XY:227:PHE:HE2	55:XY:245:ARG:HD3	1.76	0.49
1:RA:2526:G:H5'	1:RA:2742:C:O2'	2.11	0.49
8:RI:72:LEU:HD12	8:RI:138:ILE:HG21	1.93	0.49
13:RR:24:GLN:HE21	13:RR:44:LEU:HG	1.77	0.49
39:QH:18:ARG:N	39:QH:18:ARG:HD2	2.26	0.49
42:QK:85:ARG:HD3	42:QK:113:PRO:HD3	1.93	0.49
55:QY:173:GLY:HA2	55:QY:176:LYS:HE3	1.94	0.49
1:YA:848:G:H2'	1:YA:849:A:C8	2.46	0.49
1:YA:1266:G:O2'	1:YA:2012:G:O6	2.22	0.49
2:YB:28:C:OP1	14:YS:36:TYR:OH	2.23	0.49
32:XA:102:G:O2'	32:XA:151:A:N3	2.35	0.49
33:XB:45:GLN:O	33:XB:49:GLU:HG2	2.12	0.49
47:XP:53:VAL:HG13	47:XP:79:VAL:HG22	1.94	0.49
1:RA:414:C:H2'	1:RA:415:A:C8	2.48	0.49
1:RA:754:C:H2'	1:RA:755:C:C6	2.47	0.49
1:RA:919:G:N2	1:RA:2269:A:OP2	2.45	0.49
1:RA:2001:A:H2'	1:RA:2002:G:C8	2.48	0.49
1:RA:2271:G:OP1	22:R0:18:ALA:HB1	2.12	0.49
6:RG:106:LEU:HA	6:RG:110:ALA:HB3	1.93	0.49
11:RP:2:LYS:HE2	11:RP:4:SER:OG	2.12	0.49
32:QA:110:C:O2'	47:QP:25:ARG:O	2.26	0.49
50:QS:63:THR:OG1	50:QS:65:ASN:ND2	2.45	0.49
1:YA:322:A:OP2	5:YF:169:ASN:HB2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:YA:589:C:H2'	1:YA:590:A:C8	2.47	0.49
1:YA:2889:C:H3'	1:YA:2891:G:H8	1.77	0.49
5:YF:18:ARG:HG2	5:YF:19:GLU:N	2.26	0.49
19:YX:53:LYS:HB3	19:YX:82:GLN:HB3	1.93	0.49
32:XA:858:G:O6	32:XA:869:G:H3'	2.12	0.49
32:XA:1305:G:H22	32:XA:1331:G:H1'	1.77	0.49
1:RA:2243:U:H2'	1:RA:2244:U:C6	2.48	0.49
3:RD:106:ILE:HD11	3:RD:144:ALA:HB2	1.94	0.49
4:RE:170:LEU:HB3	4:RE:184:VAL:HG22	1.93	0.49
6:RG:5:VAL:HG12	26:R4:25:TYR:CE1	2.48	0.49
27:R5:48:GLU:O	27:R5:60:VAL:HG21	2.12	0.49
32:QA:171:A:H2'	32:QA:172:A:C8	2.47	0.49
33:QB:187:LEU:HA	33:QB:201:ILE:HB	1.93	0.49
40:QI:108:VAL:HG12	40:QI:109:VAL:H	1.76	0.49
50:QS:3:ARG:NH1	50:QS:10:PHE:HB2	2.26	0.49
1:YA:484:C:H2'	1:YA:485:C:C6	2.47	0.49
1:YA:1357:U:H2'	1:YA:1358:G:O4'	2.11	0.49
17:YV:6:LYS:HB2	17:YV:38:LEU:HD21	1.94	0.49
32:XA:1028:C:H2'	32:XA:1033:G:H22	1.78	0.49
43:XL:86:ARG:HH11	43:XL:99:HIS:HB2	1.77	0.49
49:XR:52:PRO:HB2	49:XR:54:ARG:HG2	1.93	0.49
1:RA:2836:U:H2'	1:RA:2837:G:C8	2.48	0.49
32:QA:452:A:H4'	47:QP:72:ARG:NH1	2.28	0.49
32:QA:1065:U:H4'	32:QA:1066:C:O5'	2.11	0.49
32:QA:1148:U:H2'	32:QA:1149:C:O4'	2.11	0.49
1:YA:1055:G:H21	1:YA:1084:A:N6	2.11	0.49
1:YA:2126:A:H4'	1:YA:2127:G:O5'	2.13	0.49
32:XA:841:U:C5	32:XA:848:C:H1'	2.48	0.49
32:XA:973:G:H3'	32:XA:974:A:H5''	1.94	0.49
1:RA:706:A:H2'	1:RA:707:G:O4'	2.13	0.49
1:RA:774:A:H2'	1:RA:774:A:N3	2.27	0.49
1:RA:1689:A:H4'	32:QA:1475:G:H4'	1.94	0.49
1:RA:2889:C:H3'	1:RA:2891:G:H8	1.77	0.49
2:RB:96:U:OP2	21:RZ:14:LYS:NZ	2.46	0.49
7:RH:137:ASP:HB3	7:RH:140:LYS:HB3	1.94	0.49
16:RU:49:HIS:HA	16:RU:52:ARG:HB3	1.95	0.49
32:QA:1239:A:C4	32:QA:1298:C:N4	2.81	0.49
1:YA:607:U:OP1	5:YF:102:PRO:HA	2.13	0.49
32:XA:1035:A:H2'	32:XA:1036:G:C8	2.47	0.49
44:XM:96:LEU:C	44:XM:110:ARG:HG2	2.33	0.49
1:RA:154(B):C:H42	1:RA:171:G:H1	1.61	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:RA:1266:G:O5'	18:RW:15:ARG:NH2	2.45	0.49
1:RA:2206:G:H8	1:RA:2207:G:N7	2.11	0.49
19:RX:53:LYS:HB3	19:RX:82:GLN:HB3	1.93	0.49
32:QA:542:G:H5'	35:QD:41:GLY:HA3	1.94	0.49
41:QJ:30:SER:OG	41:QJ:81:THR:HG22	2.11	0.49
41:QJ:40:LEU:HB2	41:QJ:69:ASN:HB2	1.95	0.49
1:YA:1069:A:O2'	1:YA:1072:C:OP1	2.27	0.49
1:YA:2119:A:N6	1:YA:2168:G:H21	2.10	0.49
1:YA:2162:G:O3'	1:YA:2172:U:O2'	2.28	0.49
1:YA:2864:G:OP1	15:YT:119:LYS:HE3	2.13	0.49
23:Y1:64:ALA:HA	23:Y1:67:ILE:HG13	1.94	0.49
26:Y4:59:PHE:CA	26:Y4:61:ARG:H	2.12	0.49
32:XA:995:C:H1'	45:YN:4:LYS:HE2	1.94	0.49
1:RA:721:C:H2'	1:RA:722:A:C8	2.48	0.49
1:RA:1693:U:O2'	3:RD:14:ARG:NH2	2.46	0.49
1:RA:1889:A:O2'	1:RA:2087:G:H5'	2.12	0.49
12:RQ:55:VAL:HG12	12:RQ:64:ILE:HD12	1.95	0.49
20:RY:6:HIS:HE1	20:RY:72:VAL:O	1.95	0.49
32:QA:1441:G:O2'	32:QA:1460:A:N6	2.46	0.49
33:QB:162:ILE:O	33:QB:185:ILE:HG12	2.13	0.49
40:QI:24:GLY:HA2	40:QI:59:PHE:O	2.13	0.49
1:YA:300:A:H2'	1:YA:334:C:H1'	1.93	0.49
8:YI:114:LEU:HD12	8:YI:116:LEU:HB2	1.95	0.49
32:XA:512:U:H2'	32:XA:513:C:C6	2.48	0.49
32:XA:1435:G:H2'	32:XA:1436:U:C6	2.48	0.49
35:XD:25:ARG:NH1	35:XD:30:LYS:O	2.45	0.49
36:XE:6:PHE:HB2	36:XE:34:VAL:HG13	1.94	0.49
55:XY:107:ASP:O	55:XY:173:GLY:N	2.35	0.49
55:XY:228:ARG:HD3	55:XY:238:ASN:O	2.12	0.49
1:RA:1569:A:H2'	1:RA:1570:A:C8	2.48	0.49
1:RA:2343:C:O2'	1:RA:2373:G:O2'	2.14	0.49
32:QA:426:G:OP1	35:QD:38:TYR:OH	2.24	0.49
32:QA:1305:G:N2	32:QA:1331:G:H1'	2.28	0.49
36:QE:8:GLU:OE2	36:QE:63:ARG:NH2	2.46	0.49
1:YA:922:U:H2'	1:YA:923:C:C6	2.48	0.49
1:YA:2836:U:H2'	1:YA:2837:G:C8	2.48	0.49
16:YU:92:ARG:HA	16:YU:95:LEU:HB2	1.95	0.49
32:XA:36:C:OP1	43:XL:123:LYS:HE2	2.13	0.49
32:XA:189(M):G:H2'	32:XA:190:U:C6	2.48	0.49
32:XA:457:C:H2'	32:XA:458:C:H6	1.78	0.49
32:XA:1403:C:H1'	32:XA:1500:A:N1	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:XD:116:GLN:NE2	35:XD:157:LEU:HD11	2.27	0.49
40:XI:31:GLN:HG3	40:XI:36:TYR:HB2	1.95	0.49
1:RA:826:U:H2'	1:RA:828:U:O4'	2.13	0.48
1:RA:1045:A:H4'	1:RA:1046:A:C5'	2.44	0.48
14:RS:48:LEU:HD23	14:RS:82:ILE:HD11	1.95	0.48
19:RX:5:TYR:O	24:R2:36:ARG:NH2	2.42	0.48
32:QA:890:G:O2'	32:QA:906:G:O6	2.28	0.48
33:QB:115:LEU:HD12	33:QB:142:LEU:HD12	1.94	0.48
35:QD:106:TYR:HE2	35:QD:107:ARG:HH11	1.61	0.48
36:QE:74:GLY:HA3	36:QE:116:THR:HG22	1.95	0.48
1:YA:1525:G:H2'	1:YA:1526:G:C8	2.48	0.48
1:YA:1971:A:C4	3:YD:241:PRO:HD3	2.48	0.48
1:YA:2389:G:H5''	1:YA:2390:U:O4'	2.13	0.48
4:YE:119:ARG:HD3	4:YE:120:TRP:NE1	2.28	0.48
6:YG:115:ARG:HG3	6:YG:136:ARG:HH21	1.78	0.48
9:YN:108:PRO:O	9:YN:113:GLY:HA3	2.13	0.48
26:Y4:40:HIS:HB3	26:Y4:43:TYR:CD1	2.48	0.48
32:XA:1129:C:H2'	32:XA:1139:G:N7	2.28	0.48
32:XA:1346:A:OP1	40:XI:120:ARG:NH1	2.34	0.48
55:XY:123:GLU:CG	55:XY:188:PRO:HB3	2.43	0.48
1:RA:214:G:H1'	1:RA:216:A:O2'	2.13	0.48
4:RE:178:GLU:H	4:RE:178:GLU:CD	2.15	0.48
1:YA:272(E):U:H2'	1:YA:272(F):C:C6	2.48	0.48
1:YA:438:G:H2'	1:YA:440:G:C8	2.48	0.48
1:YA:1826:G:H4'	3:YD:242:ARG:CZ	2.43	0.48
26:Y4:48:ARG:HG3	26:Y4:52:THR:HG23	1.93	0.48
32:XA:149:A:H2'	32:XA:150:C:C6	2.48	0.48
34:XC:125:GLU:OE1	34:XC:190:ARG:NH1	2.46	0.48
1:RA:539:G:H2'	1:RA:540:C:H6	1.78	0.48
1:RA:2704:C:H2'	1:RA:2705:A:O4'	2.13	0.48
15:RT:35:LYS:HD3	15:RT:40:THR:HG22	1.94	0.48
32:QA:184:G:H2'	32:QA:185:A:H8	1.78	0.48
51:QT:63:ILE:HG21	51:QT:81:LYS:HG3	1.96	0.48
1:YA:1053:C:H2'	1:YA:1054:A:C8	2.49	0.48
1:YA:2321:G:O2'	1:YA:2322:A:OP1	2.23	0.48
5:YF:185:ASP:OD1	5:YF:188:ARG:NH1	2.46	0.48
10:YO:38:VAL:HG13	10:YO:87:ILE:HD11	1.94	0.48
40:XI:31:GLN:HB2	40:XI:35:GLU:HG2	1.95	0.48
43:XL:117:ARG:HG2	43:XL:122:THR:HB	1.96	0.48
1:RA:856:C:H2'	1:RA:857:C:C6	2.49	0.48
1:RA:1259:G:H2'	1:RA:1260:G:H8	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:RA:2142:C:H2'	1:RA:2143:C:C6	2.48	0.48
1:RA:2466:C:OP1	31:R9:4:ARG:HB2	2.13	0.48
4:RE:119:ARG:HH21	4:RE:158:GLY:N	2.11	0.48
11:RP:100:LEU:HD12	11:RP:112:LEU:HD11	1.95	0.48
14:RS:20:ARG:O	14:RS:20:ARG:HD3	2.12	0.48
21:RZ:198:LYS:HB2	21:RZ:203:GLU:HA	1.96	0.48
24:R2:65:ASN:OD1	24:R2:69:ARG:NH1	2.40	0.48
32:QA:115:G:H4'	32:QA:116:A:O5'	2.13	0.48
32:QA:184:G:H2'	32:QA:185:A:C8	2.49	0.48
35:QD:25:ARG:NH1	35:QD:30:LYS:O	2.47	0.48
51:QT:42:GLN:NE2	51:QT:46:GLU:OE2	2.47	0.48
1:YA:1404:C:H2'	1:YA:1405:U:H6	1.78	0.48
7:YH:56:SER:OG	7:YH:58:GLU:HG2	2.13	0.48
11:YP:98:GLU:OE1	11:YP:98:GLU:N	2.40	0.48
20:YY:99:CYS:SG	20:YY:100:ALA:N	2.87	0.48
21:YZ:10:ARG:NH2	21:YZ:26:GLY:O	2.43	0.48
32:XA:715:A:H2'	32:XA:716:A:C8	2.48	0.48
33:XB:145:LEU:HD12	33:XB:149:LEU:HD12	1.95	0.48
1:RA:764:A:O4'	3:RD:213:ARG:HG3	2.13	0.48
1:RA:1250:G:N7	11:RP:18:ARG:NH2	2.61	0.48
1:RA:2023:G:H4'	1:RA:2617:C:O3'	2.14	0.48
9:RN:58:ASP:N	9:RN:58:ASP:OD1	2.47	0.48
32:QA:49:U:C2	32:QA:361:G:N2	2.82	0.48
32:QA:1003:G:C2'	32:QA:1004:A:H4'	2.44	0.48
32:QA:1068:G:OP2	32:QA:1068:G:H8	1.96	0.48
32:QA:1359:C:H4'	32:QA:1362:C:H41	1.79	0.48
47:QP:17:TYR:HE2	47:QP:41:PRO:HG3	1.78	0.48
53:QV:16:C:O2'	53:QV:61:C:OP1	2.27	0.48
7:YH:159:GLU:HG3	7:YH:169:VAL:HG11	1.95	0.48
18:YW:29:LEU:HD22	18:YW:69:LEU:HD12	1.96	0.48
35:XD:64:LEU:HB2	35:XD:198:VAL:HG11	1.95	0.48
1:RA:1021:A:O2'	1:RA:1123:C:OP1	2.20	0.48
1:RA:1721:G:N1	1:RA:1739:U:OP2	2.46	0.48
4:RE:119:ARG:HG3	4:RE:160:TYR:HB2	1.94	0.48
11:RP:86:LYS:HB3	11:RP:118:GLY:HA3	1.95	0.48
14:RS:27:SER:HA	14:RS:88:ASP:HB3	1.94	0.48
32:QA:1187:G:H4'	40:QI:111:ARG:NH1	2.28	0.48
37:QF:97:PHE:HB2	49:QR:32:ARG:HH11	1.79	0.48
40:QI:3:GLN:OE1	40:QI:20:ARG:NH2	2.29	0.48
49:QR:33:ASP:OD2	49:QR:36:ASN:HB2	2.13	0.48
1:YA:626:U:O4	11:YP:107:LYS:HE2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:YI:72:LEU:HD21	8:YI:107:VAL:HG11	1.95	0.48
18:YW:14:PRO:HG2	18:YW:78:GLU:HG3	1.95	0.48
21:YZ:198:LYS:CE	53:XV:52:G:H2'	2.37	0.48
32:XA:444:C:H42	32:XA:490:G:H1	1.61	0.48
32:XA:473:G:OP2	47:XP:75:ARG:HD3	2.14	0.48
32:XA:1003:G:H3'	32:XA:1003:G:N3	2.29	0.48
32:XA:1258:G:H2'	32:XA:1259:C:C6	2.48	0.48
32:XA:1442(A):G:H2'	32:XA:1442(A):G:N3	2.29	0.48
53:XV:17:C:H5	53:XV:17(A):U:C5	2.32	0.48
53:XV:20:U:H2'	53:XV:21:A:H5'	1.95	0.48
1:RA:464:U:H2'	1:RA:465:G:O4'	2.14	0.48
1:RA:796:C:H2'	1:RA:797:C:C6	2.48	0.48
32:QA:750:G:O2'	46:QO:22:THR:O	2.21	0.48
32:QA:1183:A:O2'	32:QA:1184:G:OP1	2.28	0.48
32:QA:1291:G:OP1	38:QG:37:ASN:ND2	2.47	0.48
1:YA:572:A:H2'	1:YA:573:G:O4'	2.14	0.48
1:YA:652(U):C:H2'	1:YA:652(V):G:C8	2.49	0.48
1:YA:1091:G:H2'	1:YA:1091:G:N3	2.28	0.48
1:YA:1364:G:N7	23:Y1:3:LYS:HD2	2.29	0.48
1:YA:1636:C:H2'	1:YA:1637:A:C8	2.48	0.48
1:YA:1669:A:O2'	1:YA:2549:G:H5'	2.12	0.48
42:XK:27:ASN:OD1	42:XK:28:THR:N	2.46	0.48
1:RA:93:G:H2'	1:RA:94(A):C:C6	2.48	0.48
1:RA:2602:A:C5	55:QY:237:VAL:HG23	2.49	0.48
18:RW:4:LYS:HG2	18:RW:5:ALA:N	2.29	0.48
32:QA:186:C:H2'	32:QA:187:C:C6	2.49	0.48
32:QA:266:G:H2'	32:QA:266:G:N3	2.29	0.48
32:QA:1179:A:OP2	40:QI:93:ARG:NH2	2.47	0.48
55:QY:172:TYR:CE1	55:QY:207:PRO:HD3	2.49	0.48
1:YA:1645:G:H5''	1:YA:1646:C:H5'	1.94	0.48
1:YA:1991:U:H2'	1:YA:1992:G:H5''	1.95	0.48
32:XA:407:G:OP1	35:XD:115:ARG:NH2	2.37	0.48
1:RA:1022:G:C5	1:RA:1140:C:C4	3.01	0.48
1:RA:1639:U:C2'	1:RA:1640:C:H5''	2.43	0.48
1:RA:2296:U:OP2	14:RS:9:ARG:NH2	2.42	0.48
3:RD:2:ALA:N	3:RD:200:ASP:OD2	2.47	0.48
32:QA:176:C:H2'	32:QA:177:C:C6	2.49	0.48
32:QA:520:A:N1	32:QA:536:C:H1'	2.29	0.48
32:QA:1479:C:H2'	32:QA:1480:G:H8	1.79	0.48
33:QB:96:ARG:HG2	33:QB:98:LEU:HD23	1.96	0.48
1:YA:272(P):C:H5''	8:YI:45:LYS:HD2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:YA:751:A:H5'	18:YW:90:ARG:HA	1.95	0.48
1:YA:1411:C:H2'	1:YA:1412:A:C8	2.49	0.48
7:YH:55:PRO:HG2	7:YH:61:HIS:ND1	2.29	0.48
13:YR:63:ARG:O	13:YR:67:LEU:HB2	2.13	0.48
34:XC:22:TRP:CD1	34:XC:59:ARG:HD2	2.49	0.48
1:RA:265:A:N1	1:RA:427:U:O2'	2.39	0.48
1:RA:721:C:H2'	1:RA:722:A:H8	1.79	0.48
1:RA:754:C:H2'	1:RA:755:C:H6	1.79	0.48
55:QY:191:GLU:OE2	55:QY:193:GLN:HB2	2.14	0.48
1:YA:614(A):U:H5'	1:YA:614(D):A:N6	2.28	0.48
1:YA:998:C:OP2	16:YU:92:ARG:NH2	2.46	0.48
1:YA:1493:C:C5	1:YA:2206:G:H2'	2.49	0.48
1:YA:2591:C:H2'	1:YA:2592:G:C8	2.48	0.48
4:YE:170:LEU:HD23	4:YE:184:VAL:HG11	1.96	0.48
9:YN:4:TYR:CD2	16:YU:100:VAL:HG11	2.48	0.48
12:YQ:68:ILE:HD13	12:YQ:103:MET:HE3	1.96	0.48
29:Y7:10:ARG:HG2	29:Y7:14:LYS:HD3	1.96	0.48
32:XA:804:U:H5''	32:XA:805:C:OP2	2.13	0.48
32:XA:1250:A:H2	32:XA:1353:G:H21	1.62	0.48
46:XO:17:ARG:HD3	46:XO:26:GLU:OE2	2.14	0.48
1:RA:2572:A:C8	4:RE:144:ARG:HD2	2.49	0.47
10:RO:8:LEU:HD22	10:RO:82:ASN:HB3	1.96	0.47
26:R4:41:PRO:HG3	26:R4:49:PHE:CE1	2.49	0.47
32:QA:107:G:H2'	32:QA:108:G:O4'	2.14	0.47
32:QA:486:U:H2'	32:QA:487:A:H8	1.79	0.47
32:QA:744:C:O2'	32:QA:851:G:N2	2.47	0.47
1:YA:459:U:H2'	1:YA:460:A:H8	1.79	0.47
1:YA:1405:U:H2'	1:YA:1406:U:C6	2.49	0.47
34:XC:137:ALA:HA	34:XC:140:ARG:HH11	1.79	0.47
40:XI:23:ASN:H	40:XI:23:ASN:HD22	1.62	0.47
40:XI:23:ASN:OD1	40:XI:25:LYS:HE2	2.14	0.47
1:RA:1084:A:H3'	1:RA:1085:A:H4'	1.96	0.47
1:RA:2150:U:H2'	1:RA:2151:G:C8	2.49	0.47
2:RB:66:A:N6	2:RB:109:C:H5''	2.27	0.47
21:RZ:129:SER:HB3	21:RZ:132:ASN:HB2	1.95	0.47
31:R9:27:CYS:SG	31:R9:28:GLU:N	2.87	0.47
32:QA:973:G:H3'	32:QA:974:A:H5''	1.95	0.47
32:QA:992:U:H4'	32:QA:993:G:H5'	1.95	0.47
39:QH:73:ASP:OD1	39:QH:75:ARG:HG3	2.15	0.47
1:YA:154(B):C:H42	1:YA:171:G:H1	1.62	0.47
1:YA:276:A:H5''	1:YA:277:C:H5'	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:YA:1028:A:N3	1:YA:2486:G:O2'	2.39	0.47
1:YA:1053:C:H2'	1:YA:1054:A:H8	1.79	0.47
1:YA:1798:U:H5'	3:YD:259:THR:CG2	2.39	0.47
1:YA:2032:G:H1'	4:YE:145:LYS:HD3	1.97	0.47
3:YD:177:LEU:HD11	3:YD:183:ARG:HD3	1.96	0.47
5:YF:53:THR:HG22	5:YF:56:GLU:OE2	2.13	0.47
11:YP:62:LEU:O	30:Y8:13:ARG:HD3	2.14	0.47
32:XA:148:G:H2'	32:XA:149:A:C8	2.49	0.47
32:XA:741:G:H2'	32:XA:742:G:O4'	2.14	0.47
32:XA:1179:A:H2'	32:XA:1180:A:O4'	2.14	0.47
55:XY:258:GLN:HG3	55:XY:258:GLN:O	2.14	0.47
1:RA:273(A):G:N7	1:RA:421:U:H2'	2.29	0.47
1:RA:747:U:O2	1:RA:2014:A:H1'	2.14	0.47
1:RA:1313:U:H2'	1:RA:1610:A:C2	2.49	0.47
5:RF:184:TYR:O	5:RF:188:ARG:HG3	2.14	0.47
9:RN:96:GLU:HB2	9:RN:122:VAL:HG12	1.97	0.47
32:QA:262:A:C6	32:QA:263:A:C6	3.02	0.47
32:QA:1329:A:N7	52:QU:7:ARG:NH2	2.61	0.47
32:QA:1492:A:H8	55:QY:119:THR:CG2	2.27	0.47
33:QB:78:GLN:OE1	33:QB:95:GLN:NE2	2.47	0.47
35:QD:60:GLU:HG3	35:QD:202:LEU:HD12	1.96	0.47
42:QK:62:GLN:HB2	42:QK:93:GLN:HG3	1.96	0.47
50:QS:41:VAL:HG22	50:QS:42:PRO:HD2	1.96	0.47
55:QY:244:ILE:HD12	55:QY:267:LYS:HB2	1.96	0.47
1:YA:1165:U:H2'	1:YA:1166:C:C6	2.48	0.47
1:YA:1812:A:O2'	3:YD:45:ASN:N	2.44	0.47
20:YY:6:HIS:HE1	20:YY:72:VAL:O	1.97	0.47
1:RA:251:A:C5	1:RA:252:G:H1'	2.50	0.47
1:RA:1091:G:H2'	1:RA:1091:G:N3	2.30	0.47
1:RA:2646:C:H2'	1:RA:2647:U:O4'	2.14	0.47
32:QA:1062:U:H2'	32:QA:1063:C:C6	2.49	0.47
32:QA:1232:U:H5'	40:QI:124:GLN:O	2.13	0.47
34:QC:124:ILE:HD12	34:QC:196:LEU:HD12	1.96	0.47
40:QI:25:LYS:HD3	40:QI:25:LYS:HA	1.59	0.47
1:YA:11:G:C2'	1:YA:12:U:H5'	2.44	0.47
1:YA:1055:G:H2'	1:YA:1056:G:O4'	2.15	0.47
1:YA:1164:G:H2'	1:YA:1165:U:C6	2.50	0.47
5:YF:157:VAL:HB	5:YF:194:MET:HG2	1.96	0.47
26:Y4:15:ILE:HD12	26:Y4:21:VAL:HG22	1.97	0.47
32:XA:108:G:C6	51:XT:15:ARG:HG2	2.49	0.47
32:XA:750:G:N3	46:XO:23:GLY:HA3	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:XC:19:GLU:HB3	34:XC:40:ARG:NH2	2.29	0.47
38:XG:45:ASP:O	38:XG:49:ILE:HG13	2.14	0.47
1:RA:725:G:C6	1:RA:726:G:N1	2.83	0.47
1:RA:1002:G:H2'	1:RA:1003:G:O4'	2.15	0.47
1:RA:2180:U:H2'	1:RA:2181:G:C8	2.50	0.47
1:RA:2648:C:H2'	1:RA:2649:U:H6	1.78	0.47
1:RA:2751:G:C8	7:RH:2:SER:HA	2.50	0.47
15:RT:108:ARG:HA	15:RT:111:ARG:NH1	2.29	0.47
30:R8:23:VAL:HG13	30:R8:47:LYS:HB3	1.96	0.47
32:QA:838:G:H5'	32:QA:839:U:OP2	2.14	0.47
32:QA:1347:G:O6	40:QI:10:ARG:NH2	2.47	0.47
37:QF:11:ASN:HB3	37:QF:14:LEU:HG	1.95	0.47
1:YA:774:A:H2'	1:YA:774:A:N3	2.30	0.47
1:YA:1065:U:H4'	1:YA:1066:U:C5'	2.45	0.47
1:YA:1101:U:H2'	1:YA:1102:C:C6	2.49	0.47
11:YP:63:PRO:HD3	30:Y8:27:THR:HG22	1.96	0.47
16:YU:46:ALA:O	16:YU:50:ARG:HG3	2.14	0.47
17:YV:52:VAL:HG23	17:YV:55:ALA:HB3	1.97	0.47
32:XA:1151:A:O2'	32:XA:1152:A:O5'	2.28	0.47
32:XA:1239:A:H62	32:XA:1299:A:H62	1.61	0.47
34:XC:6:HIS:HE1	34:XC:8:ILE:HB	1.79	0.47
35:XD:148:VAL:HG11	35:XD:158:ILE:HG21	1.96	0.47
36:XE:74:GLY:HA3	36:XE:116:THR:HG22	1.96	0.47
1:RA:330:A:N7	1:RA:1210:A:O2'	2.33	0.47
1:RA:1721:G:H8	1:RA:1741:A:H62	1.62	0.47
1:RA:2128:C:H5'	1:RA:2129:C:OP2	2.15	0.47
1:RA:2512:C:H2'	1:RA:2513:G:O4'	2.14	0.47
1:RA:2805:G:H2'	1:RA:2807:G:C8	2.49	0.47
32:QA:737:A:H2'	32:QA:738:C:C6	2.50	0.47
32:QA:974:A:H8	32:QA:974:A:OP1	1.97	0.47
33:QB:167:PRO:HG3	33:QB:186:ALA:HB1	1.96	0.47
36:QE:110:LEU:HD13	36:QE:118:ILE:HG21	1.97	0.47
1:YA:1899:G:H2'	1:YA:1899:G:N3	2.30	0.47
1:YA:2342:C:O2'	1:YA:2374:C:H5''	2.14	0.47
1:YA:2687:U:H2'	1:YA:2688:U:O4'	2.13	0.47
1:YA:2716:U:H2'	1:YA:2717:G:H8	1.80	0.47
32:XA:49:U:C2	32:XA:361:G:N2	2.83	0.47
32:XA:164:U:H2'	32:XA:165:C:C6	2.50	0.47
32:XA:784:C:H2'	32:XA:785:G:O4'	2.15	0.47
34:XC:137:ALA:HA	34:XC:140:ARG:NH1	2.30	0.47
55:XY:108:GLU:HA	55:XY:170:GLY:CA	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:XY:269:LYS:O	55:XY:273:VAL:HG23	2.15	0.47
1:RA:8:A:H2'	1:RA:9:U:C6	2.49	0.47
1:RA:588:U:H2'	1:RA:589:C:C6	2.50	0.47
1:RA:2051:A:H5'	1:RA:2578:G:O4'	2.14	0.47
1:RA:2153:G:H2'	1:RA:2154:G:C8	2.49	0.47
3:RD:61:LEU:O	3:RD:63:ARG:NH1	2.48	0.47
4:RE:101:ARG:HD2	4:RE:169:ASN:O	2.14	0.47
13:RR:95:THR:HG22	13:RR:116:LEU:HD23	1.97	0.47
32:QA:418:C:H2'	32:QA:419:C:C6	2.50	0.47
32:QA:555:C:H2'	32:QA:556:C:C6	2.50	0.47
32:QA:562:C:H1'	43:QL:15:ARG:HD2	1.96	0.47
32:QA:1333:A:H2'	32:QA:1334:G:O4'	2.15	0.47
44:QM:4:ILE:HD12	44:QM:57:ARG:HA	1.96	0.47
44:QM:15:VAL:HG12	44:QM:45:VAL:HG22	1.96	0.47
55:QY:228:ARG:HD3	55:QY:238:ASN:O	2.15	0.47
1:YA:662:G:H5'	11:YP:14:LYS:O	2.15	0.47
1:YA:975(B):G:H1'	1:YA:990:A:C2	2.50	0.47
1:YA:1070:A:H2'	1:YA:1071:G:C8	2.50	0.47
1:YA:1084:A:H3'	1:YA:1085:A:C4'	2.45	0.47
1:YA:1271:G:C2	1:YA:1617:C:H4'	2.50	0.47
1:YA:2298:A:H62	1:YA:2318:G:H8	1.57	0.47
3:YD:108:PRO:HD2	3:YD:111:LEU:HD12	1.96	0.47
3:YD:108:PRO:HG2	3:YD:111:LEU:HG	1.95	0.47
15:YT:39:ARG:NH2	32:XA:345:C:OP2	2.29	0.47
27:Y5:48:GLU:O	27:Y5:60:VAL:HG11	2.15	0.47
29:Y7:12:ARG:NH2	29:Y7:44:PRO:HB3	2.30	0.47
32:XA:691:G:H1'	32:XA:696:A:N6	2.30	0.47
32:XA:902:G:H2'	32:XA:903:G:H8	1.79	0.47
32:XA:1036:G:H2'	32:XA:1037:C:O4'	2.14	0.47
32:XA:1366:C:HO2'	41:XJ:60:ARG:HH22	1.56	0.47
32:XA:1512:U:H2'	32:XA:1513:A:H8	1.80	0.47
47:XP:59:TRP:HA	47:XP:62:VAL:HG12	1.97	0.47
55:XY:287:GLN:HA	55:XY:290:GLU:HB2	1.95	0.47
1:RA:1796:U:H2'	1:RA:1797:C:H6	1.79	0.47
1:RA:2022:U:O2'	1:RA:2617:C:H5'	2.14	0.47
9:RN:97:ARG:HA	9:RN:100:GLU:HB2	1.97	0.47
23:R1:53:VAL:HG22	23:R1:74:VAL:HG13	1.97	0.47
32:QA:1151:A:O2'	32:QA:1152:A:H8	1.98	0.47
1:YA:248:G:H5'	1:YA:250:G:N7	2.29	0.47
4:YE:143:ASN:HD22	4:YE:147:PRO:HD3	1.80	0.47
6:YG:7:LEU:HD23	6:YG:100:TRP:HE3	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:YI:4:ILE:HD11	8:YI:44:LEU:HD12	1.97	0.47
26:Y4:48:ARG:HB3	26:Y4:52:THR:HA	1.96	0.47
32:XA:922:G:H4'	36:XE:20:GLN:HA	1.96	0.47
33:XB:178:ARG:HH22	39:XH:74:PRO:HB3	1.79	0.47
35:XD:79:PHE:CE1	35:XD:204:ILE:HD13	2.50	0.47
1:RA:2742:C:OP1	31:R9:35:ARG:HD3	2.15	0.47
11:RP:138:LEU:HD23	11:RP:145:PRO:HB3	1.95	0.47
12:RQ:38:GLU:HG3	12:RQ:127:ILE:HB	1.96	0.47
14:RS:66:ALA:O	14:RS:69:VAL:HG22	2.15	0.47
15:RT:37:GLY:HA2	15:RT:38:ASN:HA	1.67	0.47
21:RZ:203:GLU:C	53:QV:53:G:H4'	2.36	0.47
32:QA:632:A:H5'	32:QA:633:G:OP2	2.14	0.47
44:QM:80:ARG:HG2	44:QM:80:ARG:HH11	1.80	0.47
47:QP:50:LYS:HD3	47:QP:50:LYS:HA	1.64	0.47
1:YA:443:A:N7	5:YF:45:ARG:HG2	2.30	0.47
1:YA:723:G:H2'	1:YA:724:U:O4'	2.15	0.47
1:YA:1364:G:C8	23:Y1:3:LYS:HD2	2.49	0.47
1:YA:1814:G:H4'	3:YD:51:VAL:HG21	1.96	0.47
1:YA:2109:U:H2'	1:YA:2110:G:C8	2.50	0.47
1:YA:2119:A:H61	1:YA:2168:G:N2	2.12	0.47
1:YA:2272:U:H5''	1:YA:2273:A:OP1	2.14	0.47
6:YG:120:LEU:HB3	6:YG:131:TYR:OH	2.15	0.47
17:YV:14:VAL:HB	17:YV:96:ILE:HG13	1.96	0.47
21:YZ:198:LYS:HE2	53:XV:52:G:C2	2.50	0.47
32:XA:583:A:H2'	32:XA:584:G:O4'	2.15	0.47
1:RA:2128:C:N3	1:RA:2160:G:N2	2.59	0.47
1:RA:2712(A):U:H1'	1:RA:2712(B):A:C8	2.50	0.47
8:RI:38:LEU:HB2	8:RI:40:THR:HG23	1.96	0.47
15:RT:16:ARG:HD3	15:RT:19:LEU:HG	1.96	0.47
32:QA:77:G:H2'	32:QA:78:G:H5'	1.96	0.47
32:QA:164:U:H2'	32:QA:165:C:C6	2.50	0.47
32:QA:1255:G:P	41:QJ:45:ARG:HH22	2.38	0.47
41:QJ:57:LYS:HE2	41:QJ:60:ARG:NH2	2.29	0.47
55:QY:120:GLY:HA3	55:QY:124:ALA:HB2	1.97	0.47
1:YA:1316:U:H2'	1:YA:1317:A:C8	2.50	0.47
1:YA:1379:A:H4'	1:YA:1380:G:OP2	2.13	0.47
1:YA:1479:G:H1'	1:YA:1558:A:OP1	2.14	0.47
1:YA:2641:G:P	9:YN:74:ARG:HH12	2.38	0.47
33:XB:17:PHE:HD1	33:XB:18:GLY:N	2.07	0.47
33:XB:201:ILE:HG21	33:XB:214:ILE:HG21	1.97	0.47
36:XE:78:HIS:HA	39:XH:105:ARG:HG3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:RA:36:G:N3	1:RA:450:G:O2'	2.46	0.46
1:RA:1504:C:H2'	1:RA:1505:C:C6	2.50	0.46
20:RY:13:VAL:HG12	20:RY:74:PRO:HA	1.97	0.46
32:QA:1218:C:H2'	32:QA:1219:U:C6	2.50	0.46
33:QB:55:PHE:HD1	33:QB:58:ILE:HD12	1.80	0.46
37:QF:97:PHE:HB2	49:QR:32:ARG:NH1	2.31	0.46
1:YA:2884:U:H2'	1:YA:2885:C:O4'	2.15	0.46
10:YO:63:VAL:HG12	10:YO:106:LEU:HD11	1.97	0.46
32:XA:110:C:H2'	32:XA:111:G:O4'	2.15	0.46
33:XB:9:GLU:HG3	33:XB:10:LEU:H	1.81	0.46
33:XB:16:HIS:O	33:XB:18:GLY:N	2.48	0.46
40:XI:8:GLY:HA3	40:XI:76:ALA:O	2.15	0.46
1:RA:956:G:H2'	1:RA:957:A:H2'	1.97	0.46
1:RA:1913:A:N7	32:QA:1493:A:O2'	2.45	0.46
24:R2:35:LEU:HD12	24:R2:53:LEU:HD12	1.97	0.46
33:QB:115:LEU:O	33:QB:119:GLU:HG2	2.15	0.46
33:QB:163:PHE:CD1	33:QB:185:ILE:HG13	2.50	0.46
1:YA:1021:A:H3'	1:YA:1021:A:N3	2.30	0.46
1:YA:1292:U:H2'	1:YA:1293:C:C6	2.50	0.46
1:YA:1423:G:OP1	1:YA:1492:G:O2'	2.31	0.46
1:YA:1637:A:H4'	1:YA:2711:A:O2'	2.16	0.46
1:YA:2849:U:H4'	1:YA:2868:A:C2	2.51	0.46
32:XA:1101:A:H4'	32:XA:1102:A:O5'	2.15	0.46
46:XO:5:LYS:O	46:XO:9:GLN:HG2	2.15	0.46
1:RA:26:G:C6	1:RA:27:G:N1	2.83	0.46
1:RA:686:G:N2	1:RA:788:A:H61	2.14	0.46
1:RA:1388:G:H4'	1:RA:1525:G:O2'	2.14	0.46
1:RA:2134:A:C5	1:RA:2157:G:H5'	2.51	0.46
3:RD:132:PRO:HG3	3:RD:190:TYR:CE1	2.51	0.46
8:RI:130:TYR:HB3	8:RI:138:ILE:HB	1.96	0.46
12:RQ:75:THR:HG21	12:RQ:87:LYS:NZ	2.31	0.46
32:QA:1101:A:H4'	32:QA:1102:A:O5'	2.15	0.46
32:QA:1286:A:H2'	32:QA:1287:A:H4'	1.96	0.46
34:QC:188:LEU:HD23	34:QC:190:ARG:HH11	1.81	0.46
39:QH:82:HIS:NE2	39:QH:84:ARG:HG2	2.30	0.46
42:QK:20:TYR:HB2	42:QK:31:THR:HG23	1.97	0.46
43:QL:83:VAL:HG13	43:QL:100:ILE:HG23	1.97	0.46
1:YA:857:C:OP1	22:Y0:77:ARG:NH2	2.38	0.46
1:YA:919:G:N2	1:YA:2269:A:OP2	2.48	0.46
1:YA:1048:A:N6	1:YA:2751:G:H1	2.14	0.46
1:YA:1359:A:N1	1:YA:1372:U:O4	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:YA:1598:C:H2'	1:YA:1599:C:H6	1.81	0.46
1:YA:2142:C:H2'	1:YA:2143:C:C6	2.51	0.46
1:YA:2629:A:H1'	1:YA:2630:G:H5''	1.98	0.46
1:YA:2683:C:OP1	15:YT:53:ARG:NH2	2.47	0.46
4:YE:94:GLU:OE2	4:YE:177:PRO:HB3	2.16	0.46
32:XA:1342:C:H2'	32:XA:1343:G:H8	1.80	0.46
32:XA:1504:G:OP1	32:XA:1507:A:H4'	2.15	0.46
33:XB:163:PHE:CE1	33:XB:185:ILE:HG22	2.51	0.46
1:RA:143(B):C:H2'	1:RA:144:C:H6	1.81	0.46
1:RA:1430:C:H2'	1:RA:1431:U:C6	2.51	0.46
1:RA:1916:A:H2'	1:RA:1917:PSU:O4'	2.15	0.46
32:QA:1239:A:H62	32:QA:1299:A:N6	2.13	0.46
35:QD:190:ASP:HB2	35:QD:193:ASP:OD2	2.15	0.46
53:QV:51:C:H2'	53:QV:52:G:O4'	2.16	0.46
1:YA:273(A):G:N7	1:YA:421:U:H2'	2.29	0.46
32:XA:257:G:H2'	32:XA:258:G:O4'	2.16	0.46
32:XA:1030(D):G:H2'	32:XA:1030(E):A:C8	2.51	0.46
32:XA:1499:A:H1'	32:XA:1520:G:H5'	1.98	0.46
32:XA:1518:MA6:O5'	32:XA:1518:MA6:H8	2.14	0.46
41:XJ:25:GLU:O	41:XJ:29:ARG:HG2	2.15	0.46
55:XY:242:SER:CA	55:XY:263:GLN:HB3	2.36	0.46
1:RA:1379:A:H4'	1:RA:1380:G:OP2	2.16	0.46
1:RA:1625:C:H2'	1:RA:1626:G:O4'	2.15	0.46
24:R2:64:LEU:HD21	24:R2:68:ARG:HE	1.80	0.46
32:QA:486:U:H2'	32:QA:487:A:C8	2.50	0.46
32:QA:501:C:H2'	32:QA:502:G:C8	2.50	0.46
32:QA:657:G:O2'	46:QO:23:GLY:HA2	2.15	0.46
33:QB:69:LEU:HD13	33:QB:91:PRO:HB2	1.97	0.46
1:YA:813:U:H2'	1:YA:814:C:C6	2.50	0.46
1:YA:2593:U:H2'	1:YA:2594:C:C6	2.51	0.46
32:XA:727:G:N2	32:XA:730:G:OP2	2.47	0.46
44:XM:80:ARG:NH2	50:XS:65:ASN:O	2.49	0.46
1:RA:1263:U:C4	1:RA:1264:G:C6	3.03	0.46
1:RA:2304:G:H22	1:RA:2312:U:H3	1.64	0.46
1:RA:2420:C:OP1	30:R8:34:TRP:HB3	2.16	0.46
6:RG:5:VAL:HG12	26:R4:25:TYR:HE1	1.81	0.46
8:RI:90:GLY:O	8:RI:121:LYS:HE2	2.15	0.46
13:RR:29:LEU:HB3	13:RR:75:LEU:HD21	1.96	0.46
21:RZ:198:LYS:HE2	53:QV:53:G:O4'	2.16	0.46
26:R4:46:GLN:O	26:R4:48:ARG:N	2.48	0.46
32:QA:976:G:N2	32:QA:1363(A):C:OP2	2.38	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:QD:148:VAL:HG11	35:QD:158:ILE:HD12	1.97	0.46
36:QE:33:VAL:HG13	36:QE:112:LEU:HD12	1.98	0.46
39:QH:51:VAL:HG21	39:QH:60:ARG:HH11	1.81	0.46
50:QS:27:GLU:CB	50:QS:28:LYS:HG3	2.46	0.46
53:QV:76:A:H3'	55:QY:234:GLY:HA3	1.96	0.46
1:YA:1188:U:H4'	17:YV:79:VAL:HG22	1.97	0.46
1:YA:1803:A:H4'	3:YD:259:THR:HG23	1.98	0.46
32:XA:1002:G:N3	32:XA:1003:G:C8	2.84	0.46
32:XA:1030(A):C:N3	32:XA:1031:G:N2	2.63	0.46
33:XB:7:VAL:O	33:XB:217:ARG:NE	2.39	0.46
34:XC:8:ILE:HD12	34:XC:16:ARG:HD3	1.98	0.46
55:XY:175:LEU:O	55:XY:205:VAL:HG21	2.15	0.46
1:RA:1038:C:N4	1:RA:1117:G:H1	2.06	0.46
1:RA:1127:A:N7	1:RA:2488:A:O2'	2.43	0.46
1:RA:1530:C:H1'	1:RA:1531:C:OP1	2.16	0.46
1:RA:2119:A:N6	1:RA:2168:G:H21	2.13	0.46
1:RA:2397:G:H5''	23:R1:28:GLY:HA2	1.98	0.46
1:RA:2802:G:H2'	1:RA:2803:C:O4'	2.16	0.46
9:RN:4:TYR:CD2	16:RU:100:VAL:HG11	2.50	0.46
28:R6:35:GLU:HG2	28:R6:50:ARG:HD3	1.98	0.46
31:R9:24:TYR:CE2	31:R9:35:ARG:HG3	2.50	0.46
32:QA:1492:A:H4'	43:QL:47:LYS:HZ1	1.80	0.46
33:QB:124:SER:HA	33:QB:125:PRO:HA	1.68	0.46
37:QF:37:VAL:HA	37:QF:65:VAL:HG12	1.97	0.46
1:YA:1065:U:H4'	1:YA:1066:U:H5'	1.97	0.46
1:YA:1525:G:H2'	1:YA:1526:G:H8	1.80	0.46
1:YA:2347:C:OP1	28:Y6:38:LYS:NZ	2.26	0.46
9:YN:58:ASP:OD1	9:YN:58:ASP:N	2.49	0.46
32:XA:540:G:H2'	32:XA:541:G:O4'	2.16	0.46
32:XA:1376:U:H2'	32:XA:1377:A:H8	1.80	0.46
34:XC:114:PRO:O	34:XC:118:GLN:HG3	2.16	0.46
48:XQ:41:LYS:HZ3	48:XQ:92:ARG:HH21	1.64	0.46
55:XY:176:LYS:HE3	55:XY:177:PHE:CZ	2.50	0.46
1:RA:239:U:H2'	1:RA:240:G:O4'	2.16	0.46
1:RA:878:A:H3'	1:RA:879:G:H8	1.78	0.46
1:RA:1036:G:H1	1:RA:1119:C:H42	1.64	0.46
1:RA:1087:G:H2'	1:RA:1088:A:H5'	1.96	0.46
1:RA:1155:A:H5''	16:RU:55:ARG:HD3	1.98	0.46
1:RA:2291:U:O2'	1:RA:2374:C:O2	2.34	0.46
1:RA:2376:A:H2'	1:RA:2377:A:O4'	2.15	0.46
1:RA:2507:C:H5''	1:RA:2573:C:N4	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:RA:2774:C:H2'	1:RA:2775:A:O4'	2.15	0.46
30:R8:62:LEU:HB3	30:R8:65:GLU:HG2	1.96	0.46
32:QA:1492:A:H1'	54:QX:20:A:O2'	2.15	0.46
33:QB:114:ARG:HD2	33:QB:114:ARG:HA	1.84	0.46
55:QY:244:ILE:H	55:QY:266:ASN:ND2	2.14	0.46
1:YA:183:C:N4	1:YA:213:A:H61	2.13	0.46
1:YA:876:C:H2'	1:YA:877:U:O4'	2.16	0.46
1:YA:1056:G:H5''	1:YA:1057:A:H5'	1.97	0.46
1:YA:2079:U:H2'	1:YA:2080:G:O4'	2.15	0.46
7:YH:28:GLY:HA3	7:YH:79:VAL:HB	1.98	0.46
11:YP:100:LEU:HD22	11:YP:105:LEU:HD12	1.97	0.46
32:XA:114:U:H1'	32:XA:353:A:H1'	1.97	0.46
32:XA:265:G:H2'	32:XA:267:C:H5	1.80	0.46
32:XA:1218:C:H2'	32:XA:1219:U:C6	2.51	0.46
32:XA:1309:G:OP1	44:XM:88:ARG:HD3	2.15	0.46
1:RA:1104:C:H2'	1:RA:1105:U:C6	2.51	0.46
1:RA:2477:C:N4	31:R9:10:ILE:HG12	2.31	0.46
1:RA:2680:C:H5'	4:RE:189:PRO:HA	1.98	0.46
1:RA:2690:C:N4	1:RA:2713:A:H1'	2.31	0.46
20:RY:99:CYS:SG	20:RY:100:ALA:N	2.89	0.46
30:R8:23:VAL:HG11	30:R8:47:LYS:HD3	1.97	0.46
30:R8:50:LEU:HA	30:R8:50:LEU:HD23	1.79	0.46
32:QA:187:C:H5''	51:QT:86:ARG:HG3	1.98	0.46
32:QA:992:U:H2'	32:QA:1043:C:H41	1.79	0.46
32:QA:1054:C:O2	32:QA:1196:U:O2'	2.33	0.46
46:QO:82:ILE:O	46:QO:86:GLY:N	2.48	0.46
53:QV:43:A:H2'	53:QV:44:A:C8	2.51	0.46
1:YA:456:C:O2'	19:YX:68:ARG:NH1	2.44	0.46
1:YA:740:U:H2'	1:YA:741:G:H8	1.81	0.46
1:YA:752:A:OP1	29:Y7:3:ARG:NH2	2.42	0.46
1:YA:960:A:C8	1:YA:962:G:C8	3.04	0.46
1:YA:2262:U:H4'	1:YA:2328:A:C2	2.51	0.46
1:YA:2704:C:H2'	1:YA:2705:A:O4'	2.16	0.46
18:YW:97:LYS:HE2	18:YW:99:ARG:NH2	2.31	0.46
30:Y8:63:PRO:HG2	30:Y8:64:TYR:CE2	2.51	0.46
32:XA:632:A:H5'	32:XA:633:G:OP2	2.16	0.46
34:XC:130:VAL:HG21	34:XC:157:ILE:HG23	1.97	0.46
1:RA:1067:A:H4'	1:RA:1068:G:OP2	2.11	0.46
1:RA:1073:A:O2'	1:RA:1074:G:O5'	2.34	0.46
1:RA:1097:U:O2	1:RA:1097:U:H2'	2.15	0.46
1:RA:1341:U:OP2	1:RA:1394:U:O2'	2.21	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:RA:1495:A:H2'	1:RA:1496:A:C8	2.50	0.46
1:RA:1588:C:H2'	1:RA:1589:C:C6	2.51	0.46
3:RD:206:LEU:HD22	3:RD:211:ARG:HD2	1.98	0.46
12:RQ:30:GLY:HA2	12:RQ:107:ALA:HB2	1.98	0.46
32:QA:222:U:H2'	32:QA:223:U:C6	2.51	0.46
32:QA:946:A:O2'	32:QA:1333:A:N3	2.41	0.46
32:QA:1143:G:H2'	32:QA:1144:G:C8	2.51	0.46
33:QB:98:LEU:O	33:QB:101:MET:HG3	2.16	0.46
42:QK:84:VAL:HG11	42:QK:91:ARG:HD2	1.97	0.46
1:YA:1587:A:H2'	1:YA:1588:C:C6	2.51	0.46
1:YA:2321:G:HO2'	1:YA:2322:A:P	2.35	0.46
1:YA:2390:U:P	30:Y8:35:GLN:HE22	2.39	0.46
1:YA:2805:G:H2'	1:YA:2807:G:C8	2.51	0.46
32:XA:266:G:O2'	32:XA:267:C:OP2	2.30	0.46
1:RA:9:U:HO2'	1:RA:10:G:P	2.39	0.45
1:RA:78:A:H2'	1:RA:79:G:C8	2.51	0.45
1:RA:573:G:O2'	1:RA:574:C:H3'	2.15	0.45
1:RA:634:C:H2'	1:RA:635:C:C6	2.51	0.45
1:RA:1657:C:H2'	1:RA:1658:C:C6	2.51	0.45
21:RZ:109:ALA:HB3	21:RZ:145:GLU:OE1	2.16	0.45
31:R9:2:LYS:NZ	31:R9:31:LYS:O	2.37	0.45
32:QA:431:A:H2'	32:QA:432:A:O4'	2.17	0.45
32:QA:1036:G:H5''	32:QA:1037:C:C5	2.52	0.45
32:QA:1106:G:H5''	34:QC:172:ARG:HG2	1.97	0.45
33:QB:160:ASP:OD1	33:QB:160:ASP:N	2.49	0.45
50:QS:12:ASP:O	50:QS:14:HIS:N	2.42	0.45
55:QY:222:LEU:HD23	55:QY:248:HIS:HA	1.98	0.45
1:YA:2611:U:C4	27:Y5:3:LYS:HG2	2.50	0.45
5:YF:20:LEU:CD2	5:YF:21:ALA:H	2.28	0.45
7:YH:8:PRO:C	7:YH:69:ARG:HH12	2.19	0.45
55:XY:227:PHE:CE2	55:XY:245:ARG:HD3	2.51	0.45
1:RA:768:G:O2'	1:RA:1379:A:N1	2.37	0.45
1:RA:827:U:O2	1:RA:2246:G:H4'	2.16	0.45
1:RA:1179:C:H2'	1:RA:1180:C:C6	2.51	0.45
1:RA:1930:G:N2	1:RA:1968:G:H2'	2.32	0.45
1:RA:1942:5MC:H4'	55:QY:257:CYS:SG	2.55	0.45
19:RX:2:LYS:NZ	19:RX:38:GLU:OE2	2.38	0.45
28:R6:6:ARG:NH1	28:R6:26:ASN:HB2	2.30	0.45
32:QA:580:U:H2'	32:QA:581:G:O4'	2.16	0.45
32:QA:786:G:H2'	32:QA:787:A:O4'	2.16	0.45
34:QC:88:ARG:NH2	34:QC:101:LEU:O	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:YA:195:A:OP1	11:YP:46:LYS:NZ	2.40	0.45
1:YA:277:C:H1'	1:YA:278:A:P	2.56	0.45
1:YA:2689:U:H4'	1:YA:2690:C:H5'	1.97	0.45
1:YA:2756:U:OP2	31:Y9:19:ARG:NH2	2.48	0.45
4:YE:51:PHE:O	4:YE:77:ILE:N	2.45	0.45
32:XA:31:G:O2'	32:XA:48:C:N4	2.49	0.45
33:XB:16:HIS:HB2	33:XB:204:ASN:HB3	1.97	0.45
35:XD:163:GLU:O	35:XD:166:LYS:HG2	2.16	0.45
47:XP:17:TYR:HE1	47:XP:41:PRO:HG3	1.82	0.45
1:RA:751:A:H5'	18:RW:90:ARG:HA	1.98	0.45
1:RA:2224:G:H4'	1:RA:2226:C:C2	2.50	0.45
1:RA:2390:U:O2'	1:RA:2391:G:H5'	2.16	0.45
1:RA:2629:A:H1'	1:RA:2630:G:H5''	1.98	0.45
3:RD:148:GLU:HB2	3:RD:151:LYS:HD2	1.99	0.45
4:RE:7:VAL:HG13	4:RE:27:LEU:HB3	1.98	0.45
8:RI:133:HIS:ND1	8:RI:134:PRO:O	2.49	0.45
15:RT:11:GLU:O	15:RT:15:VAL:HG23	2.16	0.45
17:RV:40:LEU:HB2	17:RV:46:VAL:HG12	1.98	0.45
28:R6:6:ARG:NE	28:R6:24:GLU:OE1	2.43	0.45
1:YA:857:C:N4	1:YA:858:U:O4	2.49	0.45
1:YA:2832:U:O4	1:YA:2883:A:H5''	2.16	0.45
26:Y4:15:ILE:HB	26:Y4:32:TYR:CD1	2.52	0.45
32:XA:1029:C:N4	32:XA:1030(A):C:H41	2.14	0.45
34:XC:12:LEU:HD11	45:YN:51:GLY:HA2	1.98	0.45
44:XM:97:PRO:N	44:XM:110:ARG:HG2	2.31	0.45
1:RA:1557:C:H5''	1:RA:1558:A:OP2	2.17	0.45
1:RA:1907:G:C6	1:RA:1908:C:C4	3.04	0.45
1:RA:2357:U:P	22:R0:20:ARG:HH11	2.40	0.45
1:RA:2552:2MU:C2	1:RA:2554:U:H5'	2.46	0.45
5:RF:110:LEU:HA	5:RF:110:LEU:HD23	1.77	0.45
5:RF:178:PRO:HB2	5:RF:201:VAL:CG2	2.47	0.45
26:R4:34:GLU:H	26:R4:34:GLU:HG2	1.41	0.45
32:QA:1297:C:O2'	38:QG:114:ARG:NH2	2.50	0.45
33:QB:16:HIS:CG	33:QB:17:PHE:N	2.84	0.45
37:QF:61:LEU:HD23	37:QF:63:TYR:OH	2.17	0.45
1:YA:70:G:H5''	1:YA:112:U:O2	2.17	0.45
1:YA:492:A:H2'	1:YA:493:G:O4'	2.15	0.45
1:YA:779:U:OP1	3:YD:49:ILE:HG13	2.16	0.45
1:YA:1041:C:N4	1:YA:1114:G:H1	2.10	0.45
1:YA:1092:C:OP2	1:YA:1092:C:H6	1.99	0.45
1:YA:2261:C:OP1	22:Y0:19:LYS:NZ	2.36	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:XA:142:G:H2'	32:XA:143:A:C8	2.50	0.45
32:XA:187:C:H2'	32:XA:188:C:H6	1.82	0.45
32:XA:1237:C:O3'	32:XA:1300:G:N2	2.45	0.45
1:RA:27:G:O2'	1:RA:28:A:OP2	2.30	0.45
1:RA:184:C:H2'	1:RA:185:U:C6	2.51	0.45
1:RA:1223:G:N2	1:RA:1226:A:OP2	2.44	0.45
1:RA:1418:G:H8	1:RA:1418:G:O5'	1.99	0.45
1:RA:1490:A:O2'	3:RD:99:ASP:OD1	2.34	0.45
1:RA:1826:G:H4'	3:RD:242:ARG:CZ	2.46	0.45
1:RA:2133:G:N2	1:RA:2157:G:H2'	2.31	0.45
1:RA:2810:A:N6	1:RA:2891:G:O2'	2.39	0.45
3:RD:72:LYS:HG3	3:RD:103:ARG:HH22	1.81	0.45
3:RD:242:ARG:HD3	3:RD:242:ARG:N	2.31	0.45
18:RW:18:ARG:NH1	18:RW:76:VAL:O	2.49	0.45
31:R9:25:VAL:O	31:R9:33:LYS:HA	2.17	0.45
32:QA:629:G:H2'	32:QA:630:G:O4'	2.17	0.45
32:QA:1316:G:H5''	45:QN:17:LYS:NZ	2.32	0.45
34:QC:148:GLY:HA3	34:QC:172:ARG:O	2.16	0.45
1:YA:1112:G:H2'	1:YA:1112:G:N3	2.31	0.45
1:YA:1493:C:N4	1:YA:2206:G:O2'	2.49	0.45
1:YA:1638:C:H2'	1:YA:1639:U:O4'	2.16	0.45
5:YF:150:GLY:HA2	5:YF:172:TRP:CD2	2.52	0.45
8:YI:50:ARG:O	8:YI:54:GLN:HG2	2.17	0.45
26:Y4:61:ARG:NH2	50:XS:9:VAL:HG11	2.32	0.45
35:XD:10:ARG:HB2	35:XD:40:PRO:HG3	1.99	0.45
1:RA:2643:G:H2'	1:RA:2644:G:O4'	2.17	0.45
2:RB:41:U:H5	6:RG:70:VAL:O	1.99	0.45
5:RF:10:PRO:HB3	5:RF:17:ARG:HE	1.80	0.45
16:RU:92:ARG:HA	16:RU:95:LEU:HB2	1.99	0.45
32:QA:1060:C:C5	34:QC:2:GLY:HA3	2.52	0.45
33:QB:178:ARG:NH2	33:QB:198:ASP:OD1	2.49	0.45
37:QF:19:LEU:HD11	37:QF:59:TYR:CE2	2.52	0.45
42:QK:27:ASN:OD1	42:QK:28:THR:N	2.49	0.45
1:YA:674:G:H1'	5:YF:74:ARG:HD3	1.99	0.45
1:YA:1050:A:H2'	1:YA:1051:G:C8	2.50	0.45
1:YA:2306:C:C4	1:YA:2307:G:C6	3.05	0.45
1:YA:2808:U:H5''	1:YA:2891:G:O6	2.16	0.45
3:YD:19:ALA:HB2	3:YD:204:ILE:HD11	1.99	0.45
4:YE:35:GLN:OE1	4:YE:66:HIS:HE1	1.99	0.45
4:YE:120:TRP:CD1	4:YE:155:LYS:HB3	2.51	0.45
32:XA:625:G:H4'	47:XP:16:HIS:CD2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:XE:110:LEU:HD13	36:XE:118:ILE:HG21	1.98	0.45
40:XI:6:GLY:HA3	40:XI:83:ARG:HB2	1.97	0.45
41:XJ:57:LYS:HE3	41:XJ:60:ARG:NH2	2.31	0.45
43:XL:57:LYS:HD3	43:XL:65:GLU:OE2	2.15	0.45
51:XT:57:ARG:HH12	51:XT:100:ILE:HB	1.81	0.45
1:RA:329:G:H8	1:RA:329:G:OP1	2.00	0.45
1:RA:1030:G:OP2	12:RQ:128:LYS:NZ	2.38	0.45
1:RA:1889:A:N1	1:RA:2234:G:H1'	2.32	0.45
1:RA:2695:C:H2'	1:RA:2696:U:C6	2.52	0.45
8:RI:72:LEU:C	8:RI:74:ASN:H	2.20	0.45
10:RO:10:VAL:HG21	10:RO:16:ALA:HB3	1.99	0.45
12:RQ:34:LEU:HB2	12:RQ:118:LEU:HD22	1.99	0.45
13:RR:44:LEU:HD22	13:RR:48:VAL:HG23	1.99	0.45
32:QA:411:A:OP2	35:QD:25:ARG:NH2	2.50	0.45
32:QA:1201:A:H1'	32:QA:1202:G:OP2	2.16	0.45
46:QO:21:ASP:OD1	46:QO:24:SER:HB3	2.17	0.45
1:YA:530:G:N1	1:YA:2023:G:OP1	2.35	0.45
1:YA:2128:C:H5'	1:YA:2129:C:OP2	2.16	0.45
1:YA:2572:A:N7	4:YE:144:ARG:HD3	2.30	0.45
1:YA:2716:U:H2'	1:YA:2717:G:C8	2.52	0.45
3:YD:12:SER:HB3	3:YD:208:LYS:HB3	1.99	0.45
6:YG:170:ARG:NH2	6:YG:182:LYS:O	2.49	0.45
12:YQ:109:VAL:HG13	12:YQ:113:GLN:HB2	1.98	0.45
32:XA:1270:C:O2'	32:XA:1314:C:H5'	2.16	0.45
36:XE:78:HIS:ND1	39:XH:104:ARG:HD2	2.31	0.45
1:RA:676:A:H1'	1:RA:2443:C:H1'	1.99	0.45
20:RY:9:LYS:HA	20:RY:10:GLY:HA2	1.67	0.45
27:R5:8:LYS:O	27:R5:9:LYS:HD2	2.16	0.45
41:QJ:44:VAL:HG13	41:QJ:66:ARG:HD2	1.99	0.45
47:QP:59:TRP:HA	47:QP:62:VAL:HG12	1.98	0.45
55:QY:308:ARG:HD2	55:QY:310:TYR:OH	2.17	0.45
1:YA:392:C:H5''	1:YA:409:C:H5''	1.98	0.45
1:YA:428:A:H8	1:YA:428:A:OP2	2.00	0.45
1:YA:478:A:C6	1:YA:480:A:C6	3.05	0.45
1:YA:1411:C:H2'	1:YA:1412:A:H8	1.82	0.45
1:YA:1581:G:H2'	1:YA:1582:C:O4'	2.17	0.45
1:YA:2137:C:H1'	1:YA:2154:G:H22	1.82	0.45
1:YA:2331:G:O2'	22:Y0:43:THR:HG22	2.16	0.45
16:YU:108:GLU:O	16:YU:112:ARG:HG2	2.17	0.45
32:XA:814:A:H2'	32:XA:816:A:H5''	1.99	0.45
32:XA:958:A:N3	32:XA:985:C:O2'	2.44	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:XA:1023:G:H3'	32:XA:1024:G:H8	1.81	0.45
32:XA:1227:A:N3	50:XS:83:HIS:HB3	2.32	0.45
32:XA:1366:C:O2'	41:XJ:60:ARG:NH2	2.33	0.45
38:XG:12:LEU:HD12	38:XG:12:LEU:H	1.82	0.45
53:XV:40:C:H2'	53:XV:41:C:H6	1.81	0.45
55:XY:133:ARG:HG3	55:XY:134:MET:CE	2.47	0.45
55:XY:230:SER:OG	55:XY:258:GLN:NE2	2.49	0.45
55:XY:322:ILE:HG21	55:XY:347:GLU:CD	2.36	0.45
1:RA:568:U:H5'	1:RA:945:A:N6	2.31	0.45
1:RA:1378:A:P	29:R7:10:ARG:HH22	2.40	0.45
1:RA:2321:G:HO2'	1:RA:2322:A:P	2.39	0.45
5:RF:150:GLY:HA2	5:RF:172:TRP:CD2	2.51	0.45
10:RO:26:LYS:O	10:RO:30:ALA:HB2	2.17	0.45
32:QA:438:G:N1	32:QA:495:A:OP2	2.35	0.45
32:QA:946:A:H2'	32:QA:947:G:C8	2.52	0.45
32:QA:1146:A:H5'	32:QA:1147:C:OP2	2.17	0.45
37:QF:23:LYS:NZ	37:QF:42:GLU:OE2	2.36	0.45
38:QG:70:LYS:O	38:QG:138:LYS:HE2	2.16	0.45
55:QY:214:LEU:H	55:QY:215:PRO:CD	2.30	0.45
1:YA:142(B):C:H2'	1:YA:143(A):G:O4'	2.16	0.45
1:YA:615:G:OP1	5:YF:40:GLN:NE2	2.36	0.45
1:YA:818:G:H4'	1:YA:838:C:O3'	2.17	0.45
1:YA:827:U:O2'	1:YA:2068:U:C2	2.67	0.45
1:YA:1166:C:H2'	1:YA:1167:U:C6	2.52	0.45
2:YB:73:A:C4	2:YB:105:A:C2	3.05	0.45
7:YH:4:ILE:O	7:YH:69:ARG:HG2	2.17	0.45
18:YW:79:GLY:HA3	18:YW:100:THR:HG22	1.98	0.45
34:XC:8:ILE:HD12	34:XC:16:ARG:CD	2.47	0.45
39:XH:42:GLU:HG3	39:XH:109:ILE:HD13	1.98	0.45
45:YN:3:ARG:HG2	45:YN:3:ARG:HH21	1.82	0.45
47:XP:4:ILE:O	47:XP:66:PRO:HA	2.17	0.45
55:XY:112:PHE:O	55:XY:205:VAL:HA	2.17	0.45
55:XY:183:ARG:CZ	55:XY:309:THR:HG21	2.46	0.45
1:RA:856:C:O2'	1:RA:857:C:OP1	2.26	0.45
1:RA:2127:G:H2'	1:RA:2128:C:O4'	2.17	0.45
1:RA:2786:U:O2'	4:RE:62:PRO:O	2.29	0.45
3:RD:142:VAL:HG23	3:RD:193:VAL:HA	1.99	0.45
8:RI:140:LEU:HD22	8:RI:142:VAL:HG22	1.99	0.45
42:QK:79:SER:HA	42:QK:104:GLN:HB2	1.99	0.45
1:YA:190:A:N3	1:YA:679:C:O2'	2.47	0.45
1:YA:320:A:H4'	1:YA:322:A:N7	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:YA:738:G:C2	1:YA:759:G:C5	3.05	0.45
1:YA:1028:A:N6	1:YA:1125:G:H2'	2.32	0.45
1:YA:1063:G:H2'	1:YA:1063:G:N3	2.32	0.45
1:YA:1557:C:H5''	1:YA:1558:A:OP2	2.17	0.45
1:YA:2557:G:H4'	55:XY:245:ARG:NH2	2.32	0.45
5:YF:10:PRO:HB3	5:YF:17:ARG:NE	2.23	0.45
21:YZ:33:LEU:HD21	21:YZ:90:VAL:HG11	1.98	0.45
21:YZ:91:LEU:HG	21:YZ:130:PRO:HG3	1.99	0.45
32:XA:397:A:H3'	32:XA:397:A:N3	2.32	0.45
32:XA:730:G:C5	32:XA:731:G:H1'	2.51	0.45
32:XA:1349:A:H5''	40:XI:121:ARG:HB2	1.99	0.45
32:XA:1519:MA6:H8	32:XA:1519:MA6:O5'	2.16	0.45
33:XB:189:ASP:HB3	33:XB:205:ASP:H	1.81	0.45
33:XB:224:GLN:HA	33:XB:228:GLY:O	2.17	0.45
1:RA:1075:C:C2'	1:RA:1076:C:H5'	2.48	0.44
1:RA:1790:C:H2'	1:RA:1791:A:C5	2.52	0.44
1:RA:2336:A:H61	22:R0:43:THR:HG22	1.81	0.44
1:RA:2355:C:H1'	22:R0:39:ARG:NH2	2.29	0.44
32:QA:179:A:H2'	32:QA:180:U:C6	2.52	0.44
32:QA:339:C:H2'	32:QA:340:U:C6	2.52	0.44
32:QA:433:C:H2'	32:QA:434:U:H6	1.82	0.44
35:QD:178:VAL:HG12	35:QD:179:GLU:H	1.82	0.44
51:QT:18:GLN:O	51:QT:22:ARG:HG3	2.17	0.44
55:QY:319:ASP:OD2	55:QY:344:ILE:HG12	2.16	0.44
1:YA:184:C:H2'	1:YA:185:U:H6	1.82	0.44
1:YA:330:A:HO2'	1:YA:331:A:H8	1.65	0.44
11:YP:70:GLN:OE1	11:YP:70:GLN:N	2.50	0.44
21:YZ:118:GLN:N	21:YZ:173:ALA:O	2.49	0.44
32:XA:1469:G:H2'	32:XA:1470:G:H8	1.82	0.44
41:XJ:11:PHE:CE1	41:XJ:67:THR:HG22	2.51	0.44
1:RA:228:A:H8	1:RA:229:A:H5'	1.81	0.44
1:RA:1607:C:H4'	1:RA:1608:A:O5'	2.18	0.44
1:RA:2298:A:H62	1:RA:2318:G:H8	1.63	0.44
10:RO:7:TYR:O	10:RO:8:LEU:HD23	2.17	0.44
16:RU:46:ALA:O	16:RU:50:ARG:HG3	2.16	0.44
32:QA:159:G:H2'	32:QA:161:A:OP2	2.17	0.44
32:QA:1223:C:H5''	32:QA:1224:G:H5''	2.00	0.44
34:QC:9:GLY:HA2	34:QC:12:LEU:HG	1.98	0.44
55:QY:227:PHE:CE2	55:QY:245:ARG:HD2	2.52	0.44
1:YA:236:C:H2'	1:YA:237:C:C6	2.53	0.44
1:YA:518:G:H2'	1:YA:519:U:C6	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:YA:2119:A:O2'	1:YA:2120:G:H5'	2.17	0.44
1:YA:2364:C:OP1	22:Y0:55:ARG:NH1	2.50	0.44
1:YA:2630:G:H2'	1:YA:2631:G:C8	2.52	0.44
6:YG:11:TYR:OH	6:YG:33:ARG:HG2	2.17	0.44
11:YP:101:VAL:HA	11:YP:106:LEU:O	2.18	0.44
17:YV:72:VAL:HG13	17:YV:85:LYS:HB3	2.00	0.44
20:YY:37:VAL:HG21	20:YY:72:VAL:HG21	1.99	0.44
32:XA:189(L):U:H2'	32:XA:189(M):G:C8	2.52	0.44
32:XA:688:G:H2'	32:XA:689:C:H6	1.82	0.44
32:XA:921:U:O2'	36:XE:19:MET:O	2.25	0.44
42:XK:84:VAL:HG11	42:XK:91:ARG:HD2	1.98	0.44
8:RI:9:LEU:HD13	8:RI:9:LEU:HA	1.86	0.44
25:R3:3:ARG:HH11	25:R3:60:GLU:CD	2.20	0.44
25:R3:59:VAL:O	25:R3:60:GLU:HG2	2.17	0.44
32:QA:186:C:O2'	51:QT:85:MET:SD	2.66	0.44
32:QA:551:U:H2'	32:QA:552:U:C6	2.52	0.44
32:QA:786:G:C2	32:QA:797:C:C2	3.05	0.44
32:QA:1060:C:C4	34:QC:2:GLY:HA3	2.51	0.44
35:QD:79:PHE:HE1	35:QD:204:ILE:HD13	1.82	0.44
35:QD:155:LEU:O	35:QD:159:ARG:HG3	2.17	0.44
36:QE:137:GLU:OE1	36:QE:140:ARG:HD2	2.18	0.44
40:QI:22:GLY:HA3	40:QI:60:ASP:OD1	2.17	0.44
1:YA:460:A:H2'	1:YA:461:C:O4'	2.17	0.44
1:YA:910:A:C6	1:YA:911:A:C6	3.05	0.44
1:YA:1036:G:H1	1:YA:1119:C:H42	1.66	0.44
1:YA:1057:A:O2'	1:YA:1058:G:OP1	2.27	0.44
1:YA:1268:A:H2'	1:YA:1269:A:O4'	2.18	0.44
1:YA:1278:A:OP1	13:YR:36:THR:HG23	2.17	0.44
1:YA:2165:G:H2'	1:YA:2166:G:O4'	2.16	0.44
6:YG:36:LYS:HD3	6:YG:95:ARG:NH1	2.32	0.44
7:YH:20:ALA:HB1	7:YH:21:PRO:HD2	2.00	0.44
32:XA:1004:A:H5'	32:XA:1025:U:C5	2.51	0.44
32:XA:1164:G:H1	32:XA:1172:C:H42	1.63	0.44
32:XA:1315:U:H2'	32:XA:1316:G:O4'	2.17	0.44
32:XA:1372:U:H2'	32:XA:1373:G:O4'	2.18	0.44
32:XA:1513:A:H2'	32:XA:1514:C:C6	2.52	0.44
43:XL:32:PHE:HD2	43:XL:86:ARG:HB3	1.82	0.44
54:XX:20:A:N6	55:XY:190:THR:O	2.50	0.44
1:RA:68:G:H2'	1:RA:69:C:O4'	2.18	0.44
1:RA:459:U:H4'	29:R7:40:TRP:CZ3	2.52	0.44
1:RA:760:G:H2'	1:RA:761:A:O4'	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:RA:2134:A:H8	1:RA:2156:G:H21	1.64	0.44
2:RB:66:A:H61	2:RB:108:U:H2'	1.81	0.44
6:RG:115:ARG:HB3	6:RG:136:ARG:HH22	1.82	0.44
32:QA:627:G:H2'	32:QA:628:G:H8	1.81	0.44
32:QA:1225:A:H2'	32:QA:1226:C:C5	2.53	0.44
33:QB:80:ILE:HD11	33:QB:212:GLN:HB2	1.98	0.44
33:QB:166:ASP:HB3	33:QB:169:LYS:HB3	2.00	0.44
34:QC:181:ASN:HB3	34:QC:205:GLY:O	2.17	0.44
36:QE:50:GLU:HB2	36:QE:53:LEU:HD13	1.98	0.44
47:QP:19:ILE:HD11	47:QP:74:LEU:HD11	1.99	0.44
50:QS:20:LEU:HD23	50:QS:23:ASN:HD22	1.82	0.44
1:YA:272(P):C:HO2'	8:YI:42:SER:HG	1.39	0.44
1:YA:323:G:C8	5:YF:171:PRO:HG3	2.52	0.44
1:YA:1053:C:O2'	1:YA:1054:A:OP1	2.29	0.44
5:YF:101:LEU:HD12	5:YF:102:PRO:HD2	1.99	0.44
33:XB:28:PHE:O	33:XB:32:ILE:HG13	2.18	0.44
39:XH:46:LYS:HG3	39:XH:64:LYS:HB2	1.98	0.44
55:XY:349:GLN:O	55:XY:353:LEU:N	2.41	0.44
1:RA:78:A:H2'	1:RA:79:G:H8	1.82	0.44
1:RA:84:A:H5''	20:RY:8:LYS:HE2	1.98	0.44
1:RA:1178:C:P	1:RA:1178:C:H6	2.41	0.44
1:RA:1803:A:O2'	3:RD:259:THR:HG21	2.17	0.44
1:RA:1866:C:H2'	1:RA:1876:A:O4'	2.18	0.44
1:RA:2029:G:H2'	1:RA:2031:A:OP1	2.16	0.44
1:RA:2516:G:C6	1:RA:2517:C:N4	2.86	0.44
19:RX:35:THR:HB	19:RX:38:GLU:HB2	2.00	0.44
26:R4:58:ARG:HD2	50:QS:68:GLY:H	1.83	0.44
54:QX:14:A:H2'	54:QX:14:A:N3	2.31	0.44
55:QY:349:GLN:O	55:QY:353:LEU:HG	2.17	0.44
1:YA:1496:A:N3	1:YA:1577:C:O2'	2.41	0.44
1:YA:2180:U:H2'	1:YA:2181:G:C8	2.51	0.44
11:YP:97:PRO:HD3	11:YP:126:VAL:O	2.17	0.44
12:YQ:11:LYS:HE2	12:YQ:88:GLY:O	2.18	0.44
13:YR:95:THR:HG22	13:YR:116:LEU:HD23	2.00	0.44
26:Y4:58:ARG:HD3	50:XS:65:ASN:O	2.18	0.44
32:XA:828:A:H2'	32:XA:829:G:O4'	2.17	0.44
36:XE:137:GLU:OE1	36:XE:141:GLN:NE2	2.50	0.44
40:XI:53:VAL:HG11	40:XI:92:TYR:CE1	2.52	0.44
1:RA:620:G:N3	1:RA:620:G:H5'	2.32	0.44
1:RA:807:U:OP2	11:RP:41:ARG:NH2	2.51	0.44
1:RA:1045:A:H4'	1:RA:1046:A:H5'	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:RA:2342:C:O2'	1:RA:2374:C:H5''	2.18	0.44
5:RF:12:LEU:HD13	5:RF:124:LEU:HD11	1.99	0.44
12:RQ:59:ARG:HG2	12:RQ:59:ARG:HH11	1.83	0.44
16:RU:76:TYR:CZ	16:RU:80:ILE:HG13	2.53	0.44
21:RZ:91:LEU:HD12	21:RZ:91:LEU:HA	1.84	0.44
21:RZ:125:LEU:HB3	21:RZ:165:VAL:HG13	1.99	0.44
24:R2:65:ASN:O	24:R2:69:ARG:HG3	2.17	0.44
32:QA:363:A:OP1	43:QL:33:ARG:HD3	2.18	0.44
32:QA:501:C:H2'	32:QA:502:G:H8	1.81	0.44
32:QA:1442(A):G:N3	32:QA:1442(A):G:H2'	2.32	0.44
34:QC:50:ALA:HB1	34:QC:70:VAL:HG21	1.99	0.44
35:QD:156:GLU:O	35:QD:160:GLN:HG2	2.17	0.44
51:QT:101:GLY:HA2	51:QT:102:GLY:HA2	1.66	0.44
53:QV:15:G:H21	53:QV:21:A:H1'	1.82	0.44
1:YA:1025:G:C4	1:YA:1135:C:H1'	2.53	0.44
1:YA:2070:G:H2'	1:YA:2071:A:C8	2.53	0.44
1:YA:2115:G:N2	1:YA:2171:A:H61	2.14	0.44
1:YA:2712(A):U:O2'	1:YA:2712(B):A:P	2.76	0.44
6:YG:113:ARG:NH2	26:Y4:33:VAL:HG12	2.24	0.44
10:YO:68:GLU:HB3	10:YO:78:ARG:HB2	2.00	0.44
22:Y0:23:VAL:HG22	22:Y0:38:VAL:HG22	1.99	0.44
26:Y4:59:PHE:HA	26:Y4:60:GLN:C	2.38	0.44
30:Y8:52:LYS:O	30:Y8:56:GLU:HG3	2.17	0.44
32:XA:933:G:O6	38:XG:3:ARG:NH2	2.49	0.44
32:XA:1151:A:O2'	32:XA:1152:A:H8	2.01	0.44
44:XM:4:ILE:HD11	44:XM:60:VAL:HG11	1.99	0.44
1:RA:2507:C:H5''	1:RA:2573:C:H41	1.83	0.44
1:RA:2573:C:N4	55:QY:238:ASN:O	2.50	0.44
4:RE:116:VAL:HG13	4:RE:122:PHE:HB2	2.00	0.44
15:RT:28:VAL:HG13	15:RT:86:ILE:HG23	1.99	0.44
21:RZ:5:LEU:HD11	21:RZ:44:PHE:HD1	1.83	0.44
32:QA:7:G:H5''	32:QA:298:A:O4'	2.18	0.44
32:QA:297:G:N2	32:QA:300:A:OP2	2.43	0.44
34:QC:32:LEU:HD22	34:QC:59:ARG:NH1	2.32	0.44
38:QG:113:GLU:HG3	38:QG:118:VAL:HG12	2.00	0.44
39:QH:121:ASP:OD1	39:QH:121:ASP:N	2.51	0.44
1:YA:247:G:H4'	1:YA:386:G:C5	2.53	0.44
1:YA:632:A:H2'	1:YA:633:A:C8	2.53	0.44
1:YA:2467:C:H4'	12:YQ:123:HIS:CG	2.53	0.44
4:YE:112:GLY:O	4:YE:159:HIS:HA	2.17	0.44
7:YH:12:PRO:O	7:YH:15:VAL:HG22	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:Y0:26:TYR:O	22:Y0:29:GLN:HB2	2.18	0.44
26:Y4:61:ARG:NH2	50:XS:9:VAL:HG21	2.30	0.44
32:XA:410:G:P	35:XD:30:LYS:HZ1	2.40	0.44
32:XA:865:A:H2	32:XA:918:A:H4'	1.82	0.44
33:XB:174:VAL:O	33:XB:178:ARG:HG2	2.18	0.44
34:XC:148:GLY:HA3	34:XC:172:ARG:O	2.18	0.44
40:XI:26:VAL:HA	40:XI:61:ALA:O	2.18	0.44
42:XK:48:ILE:HD13	42:XK:48:ILE:HA	1.86	0.44
50:XS:62:ILE:HA	50:XS:66:MET:SD	2.57	0.44
55:XY:114:GLU:HG2	55:XY:163:ILE:HG23	2.00	0.44
1:RA:522:G:H2'	1:RA:523:C:C6	2.53	0.44
1:RA:1141:U:P	9:RN:25:ARG:HH12	2.40	0.44
1:RA:1688:U:O2	1:RA:1700:A:H5'	2.18	0.44
1:RA:1721:G:H2'	1:RA:1740:G:O6	2.18	0.44
1:RA:1918:A:O2'	1:RA:1920:4OC:N4	2.51	0.44
3:RD:108:PRO:HD2	3:RD:111:LEU:HG	1.99	0.44
8:RI:62:LYS:O	8:RI:66:GLU:HG2	2.18	0.44
18:RW:84:ARG:O	18:RW:96:ILE:N	2.44	0.44
33:QB:82:ARG:HG3	33:QB:82:ARG:HH11	1.82	0.44
40:QI:16:ARG:HH11	40:QI:64:THR:HG21	1.82	0.44
1:YA:82:G:N2	1:YA:103:A:OP2	2.51	0.44
1:YA:250:G:C6	1:YA:251:A:C6	3.06	0.44
1:YA:729:G:C6	3:YD:208:LYS:HB2	2.53	0.44
1:YA:1429:G:H2'	1:YA:1430:C:C6	2.53	0.44
1:YA:2136:C:O2	1:YA:2156:G:O2'	2.27	0.44
1:YA:2314:C:H2'	1:YA:2315:G:C8	2.53	0.44
5:YF:29:ASN:HB3	5:YF:112:MET:HE1	1.99	0.44
5:YF:150:GLY:HA2	5:YF:172:TRP:CE3	2.53	0.44
6:YG:36:LYS:HB3	6:YG:95:ARG:HG2	2.00	0.44
6:YG:101:ILE:HD13	26:Y4:25:TYR:HB2	2.00	0.44
32:XA:41:G:H2'	32:XA:42:G:C8	2.52	0.44
32:XA:581:G:OP1	46:XO:61:GLY:HA3	2.18	0.44
33:XB:69:LEU:HB3	33:XB:162:ILE:HG22	1.99	0.44
1:RA:286:C:H2'	1:RA:287:C:C6	2.52	0.44
1:RA:652(C):A:N6	1:RA:655:A:H1'	2.29	0.44
1:RA:2345:G:H1'	1:RA:2382:G:H5'	2.00	0.44
6:RG:15:VAL:HG13	6:RG:175:LEU:HB3	2.00	0.44
7:RH:3:ARG:HH12	7:RH:65:HIS:HB3	1.83	0.44
10:RO:36:GLY:HA3	10:RO:109:LYS:HD2	1.98	0.44
11:RP:63:PRO:HB2	30:R8:30:ARG:NH2	2.32	0.44
26:R4:59:PHE:CE1	50:QS:64:GLU:HG3	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:QA:571:U:O2	32:QA:918:A:H5'	2.17	0.44
32:QA:1024:G:H2'	32:QA:1024:G:N3	2.32	0.44
32:QA:1031:G:C2'	32:QA:1032:G:H5'	2.48	0.44
35:QD:57:ARG:NH2	36:QE:107:ARG:HD3	2.33	0.44
35:QD:173:TRP:CE3	35:QD:174:LEU:HG	2.52	0.44
36:QE:57:LYS:HG2	36:QE:61:TYR:CE2	2.52	0.44
36:QE:90:VAL:O	36:QE:120:THR:HA	2.18	0.44
39:QH:46:LYS:HG3	39:QH:64:LYS:HB2	2.00	0.44
55:QY:191:GLU:HG2	55:QY:195:ARG:HG2	2.00	0.44
1:YA:7:G:H2'	1:YA:8:A:C8	2.53	0.44
1:YA:699:A:H2'	1:YA:700:G:O4'	2.18	0.44
1:YA:747:U:O2	1:YA:2014:A:H1'	2.17	0.44
1:YA:1097:U:O2	1:YA:1097:U:H2'	2.17	0.44
1:YA:1721:G:H5''	1:YA:1721:G:N3	2.33	0.44
5:YF:24:LEU:HD21	5:YF:114:VAL:HG12	2.00	0.44
14:YS:71:ARG:O	14:YS:75:GLU:HG2	2.18	0.44
18:YW:10:VAL:HG12	18:YW:12:ILE:HG22	2.00	0.44
23:Y1:23:LYS:HB3	23:Y1:29:GLY:HA3	2.00	0.44
25:Y3:7:LYS:HG3	25:Y3:34:GLU:HG3	2.00	0.44
32:XA:131:C:H2'	32:XA:132:C:C6	2.52	0.44
32:XA:560:U:H4'	32:XA:561:U:O5'	2.18	0.44
32:XA:688:G:H2'	32:XA:689:C:C6	2.53	0.44
32:XA:1100:C:H2'	32:XA:1102:A:O5'	2.17	0.44
32:XA:1333:A:H2'	32:XA:1334:G:O4'	2.17	0.44
33:XB:218:ALA:O	33:XB:222:ILE:HG23	2.18	0.44
38:XG:16:LEU:HD11	40:XI:45:ALA:HB2	1.99	0.44
55:XY:101:LEU:N	55:XY:103:LYS:HE3	2.28	0.44
1:RA:27:G:C4	1:RA:512:G:N2	2.86	0.43
1:RA:207:A:H2'	1:RA:208:C:O4'	2.18	0.43
1:RA:375:C:H2'	1:RA:376:C:C6	2.53	0.43
1:RA:1815:A:OP2	3:RD:54:ARG:NH2	2.50	0.43
1:RA:1916:A:H8	1:RA:1916:A:O5'	2.02	0.43
1:RA:2149:G:C2	1:RA:2150:U:H1'	2.53	0.43
1:RA:2262:U:H4'	1:RA:2328:A:C2	2.53	0.43
3:RD:182:LEU:HB2	3:RD:272:ALA:HB3	2.00	0.43
21:RZ:198:LYS:HE3	53:QV:52:G:N2	2.33	0.43
32:QA:532:A:N6	34:QC:193:TYR:HA	2.32	0.43
32:QA:881:G:P	43:QL:12:ARG:HH22	2.41	0.43
32:QA:1030(D):G:H2'	32:QA:1030(E):A:C8	2.53	0.43
32:QA:1158:C:H5	32:QA:1181:G:H1	1.64	0.43
32:QA:1438:G:H2'	32:QA:1439:C:C6	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:QM:3:ARG:HG3	44:QM:4:ILE:N	2.32	0.43
1:YA:824:A:H1'	1:YA:2358:G:N7	2.34	0.43
1:YA:1050:A:O2'	1:YA:2752:C:H4'	2.18	0.43
1:YA:1141:U:OP2	9:YN:63:THR:OG1	2.33	0.43
1:YA:2109:U:H1'	1:YA:2181:G:N2	2.32	0.43
1:YA:2313:C:H2'	1:YA:2314:C:C6	2.52	0.43
1:YA:2749:A:O3'	7:YH:62:LYS:HE3	2.18	0.43
1:YA:2893:G:H5''	1:YA:2894:G:O4'	2.18	0.43
2:YB:78:A:C2	2:YB:100:A:C4	3.06	0.43
3:YD:51:VAL:CG1	3:YD:54:ARG:HD2	2.48	0.43
3:YD:147:LEU:HD11	3:YD:183:ARG:NE	2.31	0.43
6:YG:12:TYR:HA	6:YG:16:ARG:HG2	2.00	0.43
8:YI:114:LEU:HD11	8:YI:128:LEU:HD13	2.00	0.43
9:YN:97:ARG:HA	9:YN:100:GLU:HB2	2.00	0.43
21:YZ:91:LEU:HD12	21:YZ:91:LEU:HA	1.83	0.43
32:XA:376:G:H5''	47:XP:5:ARG:HB2	2.00	0.43
32:XA:1181:G:O2'	32:XA:1182:G:N7	2.47	0.43
32:XA:1191:A:OP2	34:XC:3:ASN:ND2	2.51	0.43
33:XB:19:HIS:CG	33:XB:20:GLU:H	2.37	0.43
55:XY:225:ASP:O	55:XY:245:ARG:HB3	2.18	0.43
1:RA:1358:G:O2'	1:RA:1359:A:H5'	2.18	0.43
1:RA:2784:C:O2'	4:RE:37:ARG:NH1	2.51	0.43
11:RP:94:GLU:HG3	11:RP:124:LYS:HD3	2.00	0.43
21:RZ:158:PRO:O	21:RZ:161:VAL:HG13	2.18	0.43
32:QA:401:C:OP2	35:QD:73:ARG:NH2	2.48	0.43
32:QA:460:G:H1'	32:QA:472:A:H61	1.83	0.43
32:QA:677:U:H2'	32:QA:678:U:C6	2.53	0.43
35:QD:194:LEU:HD12	35:QD:195:ALA:H	1.83	0.43
36:QE:92:LYS:HB3	36:QE:119:LEU:HB2	2.00	0.43
1:YA:971:C:H2'	1:YA:972:G:O4'	2.19	0.43
1:YA:1112:G:C6	1:YA:1113:U:H1'	2.54	0.43
5:YF:64:ILE:HD12	5:YF:65:TRP:CZ3	2.53	0.43
32:XA:186:C:O2'	51:XT:85:MET:SD	2.71	0.43
32:XA:302:G:N3	32:XA:556:C:H4'	2.33	0.43
33:XB:16:HIS:CD2	33:XB:210:SER:HB3	2.53	0.43
33:XB:71:VAL:HG12	33:XB:93:VAL:HG22	2.00	0.43
43:XL:28:LYS:HD2	43:XL:62:SER:HB2	2.00	0.43
1:RA:839:U:H2'	1:RA:840:C:C6	2.53	0.43
1:RA:1107:G:C2	1:RA:1108:U:H1'	2.53	0.43
1:RA:1999:C:H5''	1:RA:2723:C:O2'	2.18	0.43
1:RA:2114:A:H3'	1:RA:2115:G:H8	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:RR:63:ARG:O	13:RR:67:LEU:HB2	2.18	0.43
15:RT:65:LYS:HE2	15:RT:67:SER:HB2	2.00	0.43
32:QA:1030(A):C:N3	32:QA:1031:G:N2	2.66	0.43
32:QA:1031:G:H2'	32:QA:1032:G:H5'	1.99	0.43
32:QA:1068:G:N2	32:QA:1191:A:N3	2.53	0.43
41:QJ:62:HIS:HB3	45:QN:59:ALA:HB3	2.00	0.43
47:QP:20:VAL:HG21	47:QP:32:TYR:CG	2.53	0.43
48:QQ:10:VAL:HG13	48:QQ:19:VAL:HB	2.00	0.43
1:YA:579:G:H2'	1:YA:580:C:C6	2.53	0.43
1:YA:784:A:N6	3:YD:229:VAL:HG11	2.33	0.43
1:YA:2659:G:O2'	7:YH:175:LYS:HE2	2.17	0.43
3:YD:111:LEU:HA	3:YD:111:LEU:HD23	1.74	0.43
29:Y7:33:ARG:HH11	29:Y7:33:ARG:HD2	1.69	0.43
32:XA:485:G:O2'	32:XA:486:U:OP2	2.34	0.43
32:XA:1004:A:N7	32:XA:1037:C:H2'	2.32	0.43
32:XA:1030(B):G:H2'	32:XA:1030(C):C:H5''	1.99	0.43
32:XA:1187:G:H4'	40:XI:111:ARG:HH11	1.83	0.43
32:XA:1327:C:H2'	32:XA:1328:C:H6	1.82	0.43
44:XM:22:ILE:HG21	44:XM:66:LEU:HD13	2.01	0.43
48:XQ:41:LYS:NZ	48:XQ:88:TYR:OH	2.44	0.43
1:RA:18:C:O2'	1:RA:554:U:OP1	2.34	0.43
1:RA:38:A:H2'	1:RA:39:C:C6	2.54	0.43
1:RA:108:U:H2'	1:RA:109:G:C8	2.54	0.43
1:RA:858:U:O2	1:RA:2268:A:H2'	2.19	0.43
1:RA:1449:A:N3	1:RA:1529:G:H1'	2.33	0.43
1:RA:2119:A:H61	1:RA:2168:G:N2	2.15	0.43
4:RE:73:GLU:H	4:RE:73:GLU:CD	2.21	0.43
12:RQ:61:GLY:HA2	21:RZ:177:PRO:HB2	2.00	0.43
14:RS:99:LYS:HE2	14:RS:103:GLU:OE2	2.18	0.43
26:R4:61:ARG:HG3	26:R4:62:ARG:H	1.83	0.43
32:QA:620:C:H2'	32:QA:621:A:O4'	2.19	0.43
32:QA:778:G:H2'	32:QA:779:C:O4'	2.19	0.43
43:QL:113:ARG:HH21	43:QL:116:SER:HB2	1.83	0.43
47:QP:75:ARG:HG3	47:QP:80:PHE:CD2	2.52	0.43
1:YA:64:A:O3'	19:YX:71:GLY:HA3	2.18	0.43
1:YA:785:G:C6	1:YA:786:C:C4	3.06	0.43
1:YA:2218:U:C2	23:Y1:52:ARG:NH2	2.86	0.43
17:YV:25:LEU:HD12	17:YV:94:LEU:HD21	2.00	0.43
30:Y8:23:VAL:CG1	30:Y8:47:LYS:HD3	2.48	0.43
32:XA:273:A:H1'	48:XQ:16:GLN:OE1	2.19	0.43
32:XA:404:U:C5'	35:XD:122:ARG:HD3	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:XA:790:A:C6	32:XA:791:G:C6	3.06	0.43
32:XA:1151:A:O4'	41:XJ:39:PRO:HB2	2.17	0.43
32:XA:1252:A:H2'	32:XA:1253:G:O4'	2.19	0.43
37:XF:33:TYR:HB2	37:XF:75:LEU:HD23	2.00	0.43
42:XK:16:SER:OG	42:XK:106:LYS:NZ	2.51	0.43
55:XY:144:TRP:CH2	55:XY:171:VAL:HA	2.52	0.43
1:RA:300:A:H2'	1:RA:334:C:H1'	1.99	0.43
1:RA:1864:U:OP1	1:RA:2410:G:O2'	2.21	0.43
1:RA:2245:U:H5''	1:RA:2246:G:H5'	2.01	0.43
1:RA:2869:G:H2'	1:RA:2870:C:O4'	2.18	0.43
32:QA:1027:C:H2'	32:QA:1028:C:C5	2.54	0.43
32:QA:1312:G:H5'	50:QS:5:LEU:HD12	2.01	0.43
32:QA:1315:U:H2'	32:QA:1316:G:O4'	2.18	0.43
35:QD:13:ARG:NH2	35:QD:40:PRO:HA	2.34	0.43
35:QD:107:ARG:HA	35:QD:107:ARG:HD2	1.78	0.43
43:QL:33:ARG:NH1	43:QL:62:SER:HB3	2.31	0.43
53:QV:76:A:H5''	55:QY:233:GLY:O	2.19	0.43
55:QY:114:GLU:OE1	55:QY:294:ARG:NE	2.51	0.43
1:YA:445:C:C4	1:YA:446:G:C6	3.07	0.43
1:YA:1364:G:P	23:Y1:3:LYS:HG3	2.58	0.43
1:YA:1815:A:C5	1:YA:1817:G:C6	3.05	0.43
1:YA:1936:A:OP2	1:YA:1962:5MC:N4	2.50	0.43
1:YA:2296:U:OP2	14:YS:9:ARG:NH2	2.48	0.43
1:YA:2747:G:O6	1:YA:2755:C:H5''	2.17	0.43
6:YG:165:THR:OG1	6:YG:168:GLU:HG3	2.18	0.43
7:YH:154:PRO:HB3	7:YH:163:TYR:CZ	2.53	0.43
15:YT:41:ARG:NH2	32:XA:345:C:H3'	2.33	0.43
23:Y1:3:LYS:HB2	23:Y1:61:ARG:HH11	1.84	0.43
29:Y7:24:THR:O	29:Y7:28:ARG:HG3	2.19	0.43
32:XA:269:C:H2'	32:XA:270:A:C8	2.54	0.43
32:XA:770:C:O2'	32:XA:771:G:H5'	2.18	0.43
32:XA:1342:C:H2'	32:XA:1343:G:C8	2.53	0.43
32:XA:1431:C:H2'	32:XA:1432:G:O4'	2.18	0.43
40:XI:25:LYS:HA	40:XI:25:LYS:HD3	1.77	0.43
47:XP:13:HIS:O	47:XP:42:ARG:NH1	2.52	0.43
50:XS:41:VAL:HG22	50:XS:42:PRO:HD2	1.99	0.43
1:RA:586:A:N1	1:RA:809:G:O2'	2.45	0.43
1:RA:998:C:P	16:RU:92:ARG:HH22	2.42	0.43
1:RA:2320:A:N3	1:RA:2320:A:H2'	2.33	0.43
1:RA:2724:C:OP1	4:RE:111:ARG:NH1	2.49	0.43
1:RA:2846:G:H2'	1:RA:2847:U:O4'	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:RA:2872:G:C2	1:RA:2873:A:N6	2.87	0.43
7:RH:88:LEU:HD23	7:RH:130:ARG:HG3	2.01	0.43
10:RO:3:GLN:HB2	10:RO:4:PRO:HD2	2.01	0.43
32:QA:18:C:H4'	32:QA:1078:U:O2	2.19	0.43
32:QA:840:C:H4'	32:QA:841:U:OP1	2.18	0.43
32:QA:1003:G:C2	32:QA:1004:A:N3	2.86	0.43
33:QB:115:LEU:HD13	33:QB:145:LEU:HB3	2.00	0.43
41:QJ:4:ILE:N	41:QJ:100:THR:HG22	2.33	0.43
51:QT:9:ASN:OD1	51:QT:9:ASN:N	2.50	0.43
51:QT:24:LEU:HD12	51:QT:24:LEU:HA	1.91	0.43
55:QY:170:GLY:O	55:QY:174:ARG:HG2	2.18	0.43
1:YA:117:G:C6	1:YA:119:A:C6	3.07	0.43
1:YA:1570:A:H2'	1:YA:1571:A:C8	2.53	0.43
1:YA:1802:A:C6	1:YA:1803:A:C6	3.07	0.43
1:YA:2113:U:H2'	1:YA:2114:A:O4'	2.18	0.43
8:YI:12:LEU:HD11	8:YI:25:TYR:HE2	1.84	0.43
32:XA:736:C:H2'	32:XA:737:A:H8	1.82	0.43
32:XA:881:G:P	43:XL:12:ARG:HH22	2.41	0.43
32:XA:1025:U:H3	32:XA:1036:G:H1	1.67	0.43
33:XB:8:LYS:CD	33:XB:51:LEU:HB3	2.48	0.43
43:XL:77:LEU:HD21	43:XL:107:ALA:HA	2.00	0.43
55:XY:114:GLU:HG2	55:XY:163:ILE:HG12	2.01	0.43
55:XY:114:GLU:HB2	55:XY:204:ALA:HB3	1.99	0.43
1:RA:524:U:H4'	1:RA:555:U:H4'	2.00	0.43
1:RA:527:C:N4	1:RA:2777:G:O2'	2.46	0.43
1:RA:974:G:OP1	1:RA:1187:G:O2'	2.26	0.43
1:RA:1404:C:H2'	1:RA:1405:U:H6	1.84	0.43
1:RA:2077:A:H2'	1:RA:2078:C:H6	1.83	0.43
1:RA:2352:A:N6	1:RA:2365:G:O2'	2.51	0.43
1:RA:2465:C:O2	1:RA:2486:G:C2	2.72	0.43
1:RA:2756:U:H5''	31:R9:19:ARG:HA	2.01	0.43
19:RX:12:VAL:HG21	19:RX:27:THR:HG22	2.01	0.43
27:R5:35:GLU:HG2	27:R5:51:TYR:CG	2.54	0.43
32:QA:383:A:C5	32:QA:384:G:H1'	2.54	0.43
32:QA:1356:G:H2'	32:QA:1357:A:C8	2.54	0.43
35:QD:195:ALA:O	37:XF:16:GLN:HB3	2.18	0.43
38:QG:68:ASN:O	38:QG:138:LYS:HD2	2.18	0.43
47:QP:1:MET:SD	47:QP:65:GLN:HG3	2.59	0.43
55:QY:255:VAL:HG21	55:QY:273:VAL:CG1	2.49	0.43
1:YA:185:U:H4'	1:YA:218:A:H4'	2.01	0.43
1:YA:411:G:C5	11:YP:72:PRO:HB3	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:YA:1260:G:C6	1:YA:1261:C:C4	3.07	0.43
1:YA:1287:A:O4'	13:YR:104:ARG:HD3	2.18	0.43
3:YD:275:LYS:HD2	3:YD:275:LYS:HA	1.86	0.43
4:YE:111:ARG:HG3	4:YE:160:TYR:CD2	2.54	0.43
20:YY:86:ARG:HB2	20:YY:98:VAL:HG23	2.00	0.43
24:Y2:32:LEU:HD22	24:Y2:36:ARG:HH11	1.84	0.43
32:XA:952:U:H2'	32:XA:953:G:H8	1.84	0.43
32:XA:1005:A:C5	32:XA:1006:C:H1'	2.54	0.43
33:XB:71:VAL:HG12	33:XB:93:VAL:CG2	2.49	0.43
35:XD:13:ARG:NH2	35:XD:40:PRO:HA	2.34	0.43
39:XH:84:ARG:O	39:XH:84:ARG:HG3	2.19	0.43
45:YN:27:CYS:SG	45:YN:29:ARG:HB2	2.59	0.43
1:RA:875:G:H2'	1:RA:876:C:O4'	2.18	0.43
1:RA:1084:A:H3'	1:RA:1085:A:C4'	2.48	0.43
1:RA:1188:U:H4'	17:RV:79:VAL:HG22	2.01	0.43
1:RA:2115:G:N2	1:RA:2171:A:H61	2.15	0.43
1:RA:2251:OMG:H1'	1:RA:2251:OMG:HM23	1.76	0.43
1:RA:2563:U:H2'	1:RA:2565:A:OP2	2.18	0.43
3:RD:72:LYS:HG3	3:RD:103:ARG:NH2	2.33	0.43
19:RX:88:LYS:HB2	19:RX:88:LYS:HE3	1.84	0.43
32:QA:1308:U:OP1	44:QM:98:VAL:N	2.39	0.43
35:QD:57:ARG:HD3	35:QD:205:GLU:HB3	1.99	0.43
38:QG:136:LYS:HB2	38:QG:136:LYS:HE3	1.86	0.43
47:QP:74:LEU:HB3	47:QP:79:VAL:HG21	1.99	0.43
1:YA:560:C:H5'	16:YU:52:ARG:HH21	1.84	0.43
1:YA:1486:A:H2'	1:YA:1487:G:C8	2.54	0.43
1:YA:1696:G:C6	1:YA:1697:G:C4	3.07	0.43
1:YA:2413:G:H2'	1:YA:2414:G:O4'	2.19	0.43
1:YA:2455:G:H2'	1:YA:2456:C:C6	2.53	0.43
3:YD:69:ARG:HG3	3:YD:119:ALA:HB2	2.01	0.43
32:XA:176:C:H2'	32:XA:177:C:C6	2.54	0.43
32:XA:537:G:H5''	43:XL:113:ARG:HH12	1.82	0.43
32:XA:922:G:C6	32:XA:923:A:C6	3.07	0.43
34:XC:19:GLU:HB3	34:XC:40:ARG:HH22	1.84	0.43
1:RA:388:G:OP2	23:R1:32:LYS:HG2	2.19	0.43
1:RA:470:A:H2'	1:RA:471:A:O4'	2.19	0.43
1:RA:1210:A:H5''	1:RA:1212:G:O4'	2.18	0.43
1:RA:2098:U:H2'	1:RA:2099:U:O4'	2.19	0.43
17:RV:5:VAL:HG21	17:RV:35:LEU:HD23	2.00	0.43
32:QA:447:G:H2'	32:QA:485:G:N2	2.34	0.43
33:QB:8:LYS:NZ	33:QB:52:GLU:HG3	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:QB:211:ILE:H	33:QB:211:ILE:HG13	1.65	0.43
35:QD:88:VAL:HG22	36:QE:96:PRO:HB2	2.00	0.43
35:QD:88:VAL:HG13	36:QE:97:GLY:HA2	1.99	0.43
39:QH:95:VAL:HB	39:QH:99:GLU:HG3	2.00	0.43
41:QJ:5:ARG:O	41:QJ:98:ILE:HA	2.19	0.43
1:YA:796:C:H2'	1:YA:797:C:H6	1.82	0.43
1:YA:1036:G:OP1	7:YH:59:ARG:HG2	2.18	0.43
1:YA:1040:C:H4'	21:YZ:46:LYS:HE3	2.00	0.43
1:YA:2106:G:C4	1:YA:2107:C:H1'	2.54	0.43
1:YA:2188:C:H2'	1:YA:2189:U:O4'	2.19	0.43
1:YA:2522:U:O2'	1:YA:2647:U:OP1	2.23	0.43
1:YA:2572:A:OP1	1:YA:2574:G:O2'	2.33	0.43
1:YA:2756:U:OP2	31:Y9:19:ARG:NE	2.49	0.43
5:YF:164:ARG:O	5:YF:168:ARG:HB2	2.19	0.43
7:YH:105:LEU:HD12	7:YH:105:LEU:HA	1.86	0.43
32:XA:126:G:OP1	32:XA:605:U:O2'	2.26	0.43
32:XA:501:C:H1'	32:XA:549:C:H1'	2.01	0.43
32:XA:598:U:H4'	39:XH:94:TYR:CG	2.54	0.43
32:XA:791:G:N2	32:XA:1497:G:O3'	2.51	0.43
32:XA:972:C:H4'	41:XJ:57:LYS:HB2	2.01	0.43
33:XB:28:PHE:CE1	33:XB:31:TYR:HB2	2.54	0.43
35:XD:61:LYS:NZ	35:XD:72:GLU:OE2	2.52	0.43
44:XM:54:VAL:HA	44:XM:57:ARG:HB3	2.01	0.43
55:XY:215:PRO:O	55:XY:216:ASP:C	2.57	0.43
1:RA:27:G:HO2'	1:RA:28:A:P	2.40	0.43
1:RA:284:U:H2'	1:RA:285:C:C6	2.54	0.43
1:RA:886:C:O2'	1:RA:889:C:N4	2.49	0.43
1:RA:2762:G:H2'	1:RA:2763:G:O4'	2.19	0.43
6:RG:181:ARG:HG3	6:RG:182:LYS:N	2.34	0.43
21:RZ:102:LEU:HD11	21:RZ:124:ILE:HB	2.00	0.43
24:R2:32:LEU:HD22	24:R2:36:ARG:NH1	2.34	0.43
32:QA:743:U:H2'	32:QA:744:C:C6	2.54	0.43
32:QA:943:U:H1'	40:QI:124:GLN:HE22	1.84	0.43
36:QE:145:LYS:O	36:QE:149:GLU:HG2	2.19	0.43
38:QG:26:PHE:O	38:QG:30:ILE:HG13	2.19	0.43
38:QG:104:LEU:HD12	38:QG:104:LEU:HA	1.84	0.43
47:QP:20:VAL:HG23	47:QP:35:LYS:HA	2.01	0.43
1:YA:183:C:H42	1:YA:213:A:N6	2.16	0.43
1:YA:618:C:H2'	1:YA:619:G:O4'	2.19	0.43
1:YA:2564:A:OP1	1:YA:2648:C:H4'	2.18	0.43
5:YF:63:LYS:HA	5:YF:76:GLY:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:YY:56:PRO:C	20:YY:58:GLY:H	2.22	0.43
25:Y3:43:ILE:O	25:Y3:47:VAL:HG23	2.19	0.43
32:XA:314:C:O2'	32:XA:315:A:H5'	2.19	0.43
32:XA:828:A:N6	32:XA:858:G:O2'	2.50	0.43
32:XA:1320:C:H2'	32:XA:1321:C:O4'	2.19	0.43
34:XC:9:GLY:HA3	45:XN:49:HIS:HA	2.01	0.43
37:XF:45:LEU:HD12	37:XF:59:TYR:CD2	2.54	0.43
38:XG:111:ARG:HD3	38:XG:113:GLU:OE2	2.19	0.43
1:RA:2282:G:H4'	1:RA:2389:G:O2'	2.19	0.42
1:RA:2466:C:C2	1:RA:2485:G:C2	3.07	0.42
5:RF:29:ASN:HB3	5:RF:112:MET:HE1	2.00	0.42
6:RG:108:ASN:HA	26:R4:37:SER:HB3	2.00	0.42
8:RI:109:ILE:HA	8:RI:109:ILE:HD12	1.67	0.42
9:RN:24:GLY:O	9:RN:28:THR:HG23	2.19	0.42
17:RV:81:TYR:C	17:RV:82:ARG:HD2	2.39	0.42
21:RZ:144:LEU:HD11	21:RZ:150:LEU:HD22	2.00	0.42
54:QX:21:A:C2	55:QY:196:ILE:HG23	2.54	0.42
1:YA:875:G:H2'	1:YA:876:C:O4'	2.18	0.42
1:YA:1073:A:H4'	1:YA:1074:G:OP1	2.19	0.42
1:YA:1312:U:H4'	1:YA:1313:U:O5'	2.18	0.42
1:YA:1408:C:C2	1:YA:1595:G:N2	2.87	0.42
1:YA:1889:A:H2'	1:YA:1890:A:C8	2.54	0.42
1:YA:2086:U:H2'	1:YA:2087:G:C8	2.54	0.42
5:YF:140:LEU:HD13	5:YF:170:LEU:HD21	2.00	0.42
15:YT:4:GLY:O	15:YT:8:LYS:HG2	2.19	0.42
35:XD:107:ARG:HA	35:XD:107:ARG:HD2	1.90	0.42
35:XD:200:GLU:O	35:XD:204:ILE:HG12	2.18	0.42
40:XI:22:GLY:HA3	40:XI:60:ASP:OD1	2.19	0.42
1:RA:942:G:H1'	1:RA:1189:A:C2	2.54	0.42
1:RA:1351:C:H2'	1:RA:1352:U:C6	2.54	0.42
1:RA:1422:G:C6	1:RA:1423:G:C5	3.07	0.42
1:RA:1784:A:H4'	1:RA:1785:A:O5'	2.19	0.42
1:RA:2242:G:H2'	1:RA:2243:U:O4'	2.20	0.42
3:RD:29:PRO:HB2	3:RD:34:VAL:HG11	2.00	0.42
23:R1:64:ALA:HA	23:R1:67:ILE:HG13	1.99	0.42
32:QA:612:C:O2	32:QA:629:G:N2	2.52	0.42
32:QA:1003:G:C2	32:QA:1004:A:H1'	2.54	0.42
32:QA:1055:A:O2'	34:QC:161:GLU:O	2.30	0.42
40:QI:106:ALA:O	40:QI:108:VAL:HG23	2.19	0.42
40:QI:110:GLU:OE2	40:QI:113:LYS:NZ	2.51	0.42
1:YA:26:G:C6	1:YA:27:G:N1	2.87	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:YA:45:C:OP2	1:YA:215:G:H2'	2.18	0.42
1:YA:245:G:O5'	11:YP:73:GLY:HA2	2.19	0.42
1:YA:484:C:H2'	1:YA:485:C:H6	1.83	0.42
1:YA:2106:G:C6	1:YA:2107:C:C2	3.06	0.42
1:YA:2461:C:H2'	1:YA:2462:U:C6	2.54	0.42
5:YF:21:ALA:CB	5:YF:22:ALA:HA	2.49	0.42
6:YG:72:ARG:HG2	6:YG:87:PRO:HA	2.01	0.42
23:Y1:73:LEU:HD23	23:Y1:73:LEU:HA	1.88	0.42
32:XA:409:G:H2'	32:XA:410:G:O4'	2.20	0.42
32:XA:737:A:H2'	32:XA:738:C:C6	2.54	0.42
32:XA:1376:U:H2'	32:XA:1377:A:C8	2.54	0.42
1:RA:108:U:H2'	1:RA:109:G:H8	1.84	0.42
1:RA:2267:A:H5''	1:RA:2268:A:H5'	2.02	0.42
1:RA:2438:U:O2'	1:RA:2440:C:OP1	2.26	0.42
1:RA:2462:U:H2'	1:RA:2463:C:C6	2.55	0.42
4:RE:12:THR:HG21	15:RT:11:GLU:OE2	2.19	0.42
19:RX:44:GLU:HG3	19:RX:51:VAL:HG23	2.01	0.42
26:R4:18:CYS:SG	26:R4:20:ASN:HB2	2.59	0.42
32:QA:130:A:OP2	48:QQ:63:ARG:NE	2.47	0.42
32:QA:1263:C:H2'	32:QA:1264:C:C6	2.54	0.42
33:QB:9:GLU:OE1	33:QB:217:ARG:NH2	2.45	0.42
34:QC:43:LEU:O	34:QC:47:LEU:HB2	2.19	0.42
34:QC:180:ALA:HB1	34:QC:203:PHE:CE1	2.53	0.42
36:QE:6:PHE:HD1	36:QE:36:ASP:HB3	1.83	0.42
55:QY:105:PRO:O	55:QY:107:ASP:N	2.51	0.42
55:QY:106:ASP:OD1	55:QY:109:ARG:HD2	2.19	0.42
1:YA:553:G:H2'	1:YA:554:U:O4'	2.20	0.42
1:YA:560:C:C5'	16:YU:52:ARG:HH21	2.31	0.42
1:YA:571:A:O2'	17:YV:78:LYS:HE2	2.18	0.42
1:YA:1914:C:O2	55:XY:295:ARG:HD3	2.19	0.42
1:YA:2064:C:H2'	1:YA:2065:C:C6	2.55	0.42
1:YA:2583:G:N2	55:XY:238:ASN:OD1	2.52	0.42
1:YA:2762:G:H2'	1:YA:2763:G:O4'	2.19	0.42
3:YD:5:LYS:HE3	3:YD:5:LYS:HB3	1.84	0.42
16:YU:86:ALA:O	17:YV:49:THR:HG23	2.19	0.42
32:XA:116:A:H61	32:XA:313:A:H1'	1.83	0.42
32:XA:1039:C:C4	32:XA:1040:U:C4	3.06	0.42
33:XB:8:LYS:HD2	33:XB:51:LEU:HD13	2.00	0.42
36:XE:100:VAL:O	36:XE:107:ARG:NH2	2.49	0.42
51:XT:43:LEU:HD13	51:XT:51:GLU:HB3	2.01	0.42
1:RA:10:G:H1'	1:RA:2801(B):A:N1	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:RA:569:U:C4	1:RA:570:G:C6	3.07	0.42
1:RA:631:A:H2'	1:RA:632:A:O4'	2.18	0.42
1:RA:742:G:O2'	1:RA:1676:A:H4'	2.19	0.42
1:RA:771:G:OP1	29:R7:14:LYS:HE2	2.19	0.42
1:RA:996:A:H4'	16:RU:91:ASP:OD2	2.19	0.42
1:RA:2152:G:H2'	1:RA:2153:G:H8	1.82	0.42
1:RA:2636:U:H1'	1:RA:2783:G:N2	2.34	0.42
1:RA:2712(A):U:OP1	1:RA:2714:G:H4'	2.20	0.42
1:RA:2849:U:O4	15:RT:23:ARG:NH2	2.53	0.42
3:RD:16:MET:HG3	3:RD:206:LEU:O	2.19	0.42
8:RI:4:ILE:HG12	8:RI:18:VAL:HG22	2.01	0.42
21:RZ:108:PRO:HA	21:RZ:142:SER:HA	1.99	0.42
32:QA:45:U:H2'	32:QA:46:G:H8	1.80	0.42
32:QA:399:G:H2'	32:QA:400:C:C6	2.54	0.42
32:QA:519:C:H2'	32:QA:520:A:O4'	2.20	0.42
32:QA:713:G:H2'	32:QA:714:G:C8	2.55	0.42
32:QA:1074:G:C6	32:QA:1075:C:C4	3.07	0.42
34:QC:127:ARG:CZ	34:QC:127:ARG:HB3	2.48	0.42
37:QF:23:LYS:HE2	37:QF:23:LYS:HB3	1.84	0.42
48:QQ:81:ARG:HA	48:QQ:81:ARG:HD2	1.76	0.42
55:QY:258:GLN:HG3	55:QY:258:GLN:O	2.19	0.42
1:YA:82:G:N1	1:YA:103:A:OP2	2.48	0.42
1:YA:671:C:H2'	1:YA:672:C:H6	1.84	0.42
1:YA:817:C:O2'	1:YA:839:U:H5''	2.19	0.42
1:YA:1153:C:H2'	1:YA:1154:G:O4'	2.19	0.42
1:YA:1697:G:OP2	1:YA:1698:A:O2'	2.31	0.42
1:YA:1939:5MU:O2	1:YA:1967:C:H4'	2.19	0.42
1:YA:2114:A:H3'	1:YA:2115:G:C8	2.55	0.42
1:YA:2128:C:N3	1:YA:2160:G:N2	2.63	0.42
1:YA:2193:G:H2'	1:YA:2194:G:C8	2.54	0.42
1:YA:2564:A:C2	1:YA:2647:U:H4'	2.55	0.42
1:YA:2641:G:OP1	9:YN:74:ARG:NH1	2.53	0.42
2:YB:106:G:H5'	21:YZ:31:ARG:HB3	2.01	0.42
6:YG:55:LYS:HD3	6:YG:150:ASP:OD2	2.19	0.42
18:YW:86:LEU:HD22	18:YW:96:ILE:HD11	2.01	0.42
19:YX:65:ARG:HB3	19:YX:70:LEU:HD23	2.00	0.42
32:XA:346:G:H2'	32:XA:347:G:O4'	2.19	0.42
32:XA:504:C:H1'	32:XA:510:A:C4	2.54	0.42
34:XC:180:ALA:HB1	34:XC:203:PHE:HE1	1.84	0.42
45:YN:4:LYS:HG3	45:YN:7:ILE:HD11	2.00	0.42
55:XY:317:VAL:HG23	55:XY:329:LEU:HD12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:RA:200:U:O2	1:RA:386:G:N2	2.52	0.42
1:RA:1104:C:H2'	1:RA:1105:U:H6	1.84	0.42
1:RA:2418:A:H2'	1:RA:2419:U:C6	2.55	0.42
4:RE:98:PRO:HD3	4:RE:175:VAL:HG12	2.02	0.42
5:RF:7:TYR:O	5:RF:21:ALA:HA	2.19	0.42
5:RF:165:ARG:HA	5:RF:168:ARG:CD	2.45	0.42
5:RF:178:PRO:HB2	5:RF:201:VAL:HG21	2.02	0.42
11:RP:84:ASN:HB3	11:RP:117:GLU:O	2.19	0.42
12:RQ:18:LYS:HE2	12:RQ:18:LYS:HB2	1.74	0.42
32:QA:687:A:N3	32:QA:688:G:H1'	2.34	0.42
32:QA:1015:A:H2'	32:QA:1016:A:C8	2.54	0.42
32:QA:1058:G:OP1	34:QC:199:LYS:HE3	2.20	0.42
32:QA:1075:C:OP1	33:QB:179:LYS:NZ	2.52	0.42
37:QF:6:VAL:HG22	37:QF:90:VAL:HG22	2.01	0.42
42:QK:84:VAL:CG1	42:QK:91:ARG:HD2	2.49	0.42
48:QQ:58:GLU:OE2	48:QQ:75:ARG:NH2	2.52	0.42
51:QT:63:ILE:HD13	51:QT:80:ARG:HB3	2.00	0.42
55:QY:97:GLN:O	55:QY:99:LEU:N	2.53	0.42
55:QY:222:LEU:HD21	55:QY:248:HIS:HD2	1.85	0.42
1:YA:1069:A:H2'	1:YA:1073:A:N7	2.34	0.42
1:YA:1080:C:H2'	1:YA:1081:U:C6	2.55	0.42
1:YA:1283:G:H2'	1:YA:1285:G:OP2	2.19	0.42
1:YA:2391:G:O6	1:YA:2425:A:H8	2.02	0.42
1:YA:2660:A:H2'	1:YA:2661:G:O4'	2.19	0.42
3:YD:61:LEU:O	3:YD:63:ARG:NH1	2.52	0.42
23:Y1:83:GLU:HA	23:Y1:84:GLY:HA2	1.72	0.42
32:XA:57:G:H2'	32:XA:58:C:C6	2.54	0.42
32:XA:692:U:O2'	32:XA:694:A:N7	2.41	0.42
32:XA:950:U:H2'	32:XA:951:G:C8	2.55	0.42
32:XA:1062:U:H2'	32:XA:1063:C:C6	2.54	0.42
32:XA:1063:C:H2'	32:XA:1064:G:C8	2.54	0.42
32:XA:1469:G:H2'	32:XA:1470:G:C8	2.54	0.42
33:XB:230:VAL:HG22	33:XB:231:GLU:H	1.84	0.42
40:XI:28:VAL:N	40:XI:31:GLN:O	2.45	0.42
55:XY:217:ILE:HD13	55:XY:278:ILE:CD1	2.50	0.42
1:RA:898:C:H2'	1:RA:899:A:O4'	2.20	0.42
1:RA:1264:G:N2	1:RA:2015:A:OP2	2.53	0.42
1:RA:2336:A:H61	22:R0:43:THR:CG2	2.33	0.42
1:RA:2695:C:H2'	1:RA:2696:U:H6	1.84	0.42
6:RG:114:ILE:HG12	6:RG:140:ILE:HG12	2.00	0.42
13:RR:55:ALA:HB2	13:RR:79:LEU:HD13	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:QA:110:C:H2'	32:QA:111:G:O4'	2.20	0.42
32:QA:1033:G:H2'	32:QA:1034:G:H8	1.85	0.42
32:QA:1425:U:H2'	32:QA:1426:C:C6	2.54	0.42
33:QB:141:GLU:HG2	33:QB:145:LEU:HD23	2.02	0.42
37:QF:45:LEU:HD12	37:QF:59:TYR:CD2	2.54	0.42
40:QI:65:VAL:HG21	40:QI:73:GLN:HB3	2.01	0.42
1:YA:49:A:H4'	1:YA:50:U:H5''	2.00	0.42
1:YA:305:U:H2'	1:YA:306:U:C6	2.55	0.42
1:YA:795:C:H2'	1:YA:796:C:C6	2.55	0.42
1:YA:978:G:C2	1:YA:986:C:C2	3.08	0.42
1:YA:2586:C:C5	1:YA:2608:G:N2	2.88	0.42
6:YG:114:ILE:HG23	6:YG:136:ARG:HH22	1.84	0.42
18:YW:48:ALA:O	18:YW:52:GLU:HG2	2.20	0.42
38:XG:65:ALA:HB1	38:XG:127:ALA:HB3	2.00	0.42
43:XL:89:ARG:HB3	43:XL:97:ARG:HA	2.00	0.42
55:XY:218:ASN:HA	55:XY:219:PRO:HD3	1.89	0.42
1:RA:821:A:H2'	1:RA:946:G:H5''	2.00	0.42
1:RA:962:G:H2'	1:RA:963:U:C6	2.55	0.42
1:RA:1654:A:H1'	1:RA:2823:A:H5'	2.02	0.42
1:RA:2028:U:H2'	1:RA:2029:G:O4'	2.20	0.42
1:RA:2574:G:H2'	1:RA:2575:C:O4'	2.19	0.42
5:RF:17:ARG:NH2	5:RF:19:GLU:OE2	2.53	0.42
32:QA:376:G:H5''	47:QP:5:ARG:HD3	2.01	0.42
32:QA:624:C:H2'	32:QA:625:G:H8	1.85	0.42
35:QD:76:ARG:HD2	35:QD:76:ARG:HA	1.84	0.42
39:QH:38:ILE:HD13	39:QH:41:ARG:NH2	2.35	0.42
1:YA:226:G:C2	1:YA:227:A:C6	3.07	0.42
1:YA:483:A:H1'	20:YY:59:GLY:O	2.20	0.42
1:YA:649:G:H2'	1:YA:650:C:C6	2.55	0.42
1:YA:886:C:O2'	1:YA:889:C:N4	2.52	0.42
1:YA:952:G:C6	1:YA:953:A:N7	2.88	0.42
1:YA:1019:U:OP1	1:YA:1035:U:O2'	2.25	0.42
1:YA:2193:G:H2'	1:YA:2194:G:H8	1.84	0.42
1:YA:2406:U:N3	11:YP:73:GLY:O	2.36	0.42
3:YD:182:LEU:HB2	3:YD:272:ALA:HB3	2.02	0.42
5:YF:184:TYR:O	5:YF:188:ARG:HG3	2.19	0.42
7:YH:8:PRO:HB2	7:YH:49:VAL:CG2	2.49	0.42
15:YT:53:ARG:NH1	15:YT:53:ARG:HB3	2.34	0.42
21:YZ:5:LEU:HD11	21:YZ:39:VAL:HB	2.01	0.42
32:XA:114:U:H2'	32:XA:115:G:C8	2.54	0.42
32:XA:279:A:OP2	48:XQ:95:TYR:OH	2.23	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:XA:435:C:H2'	32:XA:436:C:H6	1.84	0.42
32:XA:1104:G:H4'	33:XB:111:ARG:NH1	2.34	0.42
1:RA:458:G:O2'	1:RA:469:G:O6	2.25	0.42
1:RA:492:A:H2'	1:RA:493:G:O4'	2.20	0.42
1:RA:652(U):C:H2'	1:RA:652(V):G:C8	2.55	0.42
1:RA:984:A:H5''	1:RA:985:C:H5	1.84	0.42
1:RA:2006:C:O5'	1:RA:2006:C:H6	2.02	0.42
1:RA:2334:G:H5'	14:RS:9:ARG:HG2	2.01	0.42
1:RA:2630:G:H2'	1:RA:2631:G:C8	2.54	0.42
25:R3:3:ARG:HD3	25:R3:60:GLU:CD	2.40	0.42
32:QA:77:G:C2'	32:QA:78:G:H5'	2.49	0.42
32:QA:108:G:N1	51:QT:15:ARG:HG2	2.34	0.42
32:QA:441:A:H3'	32:QA:442:C:C6	2.55	0.42
32:QA:1125:U:H4'	41:QJ:5:ARG:NH2	2.35	0.42
32:QA:1316:G:N2	32:QA:1318:A:H3'	2.34	0.42
35:QD:53:ASP:HB3	35:QD:57:ARG:NH1	2.28	0.42
35:QD:196:LEU:H	35:QD:196:LEU:HD12	1.85	0.42
37:QF:45:LEU:HD23	37:QF:57:GLN:OE1	2.20	0.42
40:QI:4:TYR:HB2	40:QI:19:LEU:HB2	2.01	0.42
40:QI:97:LYS:HB3	40:QI:98:PRO:HD3	2.02	0.42
51:QT:10:LEU:HD23	51:QT:11:SER:H	1.84	0.42
1:YA:1040:C:H4'	21:YZ:46:LYS:CE	2.49	0.42
1:YA:1270:C:H5''	1:YA:1271:G:O5'	2.20	0.42
1:YA:1719:G:C6	1:YA:1720:U:C4	3.07	0.42
1:YA:2028:U:H2'	1:YA:2029:G:O4'	2.19	0.42
1:YA:2320:A:N3	1:YA:2320:A:H2'	2.34	0.42
30:Y8:23:VAL:HG13	30:Y8:47:LYS:HB3	2.02	0.42
32:XA:266:G:C3'	48:XQ:67:LYS:HB2	2.49	0.42
32:XA:407:G:H5''	35:XD:115:ARG:HG2	2.00	0.42
32:XA:559:A:H5''	32:XA:560:U:H3'	2.01	0.42
32:XA:601:C:H2'	32:XA:602:A:C8	2.55	0.42
32:XA:919:A:O2'	32:XA:1080:A:N1	2.38	0.42
32:XA:1009:G:H1	32:XA:1020:U:H3	1.68	0.42
38:XG:69:VAL:HG21	38:XG:104:LEU:HD11	2.02	0.42
46:XO:54:ARG:HD2	46:XO:58:MET:HE2	2.02	0.42
47:XP:60:LEU:HD12	47:XP:60:LEU:HA	1.86	0.42
53:XV:40:C:H2'	53:XV:41:C:C6	2.54	0.42
1:RA:297:C:H2'	1:RA:298:G:O4'	2.20	0.42
1:RA:579:G:H2'	1:RA:580:C:C6	2.54	0.42
1:RA:2001:A:OP1	13:RR:9:LYS:NZ	2.43	0.42
5:RF:148:LEU:CD2	5:RF:191:ARG:HE	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:RY:5:MET:HE2	20:RY:35:TYR:CD1	2.55	0.42
26:R4:24:THR:OG1	26:R4:25:TYR:N	2.53	0.42
32:QA:1427:U:H2'	32:QA:1428:A:H8	1.85	0.42
32:QA:1517:G:C6	32:QA:1518:MA6:C6	3.03	0.42
39:QH:51:VAL:HG11	39:QH:60:ARG:NH1	2.34	0.42
45:QN:27:CYS:SG	45:QN:29:ARG:HB2	2.59	0.42
50:QS:22:LEU:HD12	50:QS:31:ILE:HD11	2.02	0.42
52:QU:5:ASP:O	52:QU:11:GLY:HA3	2.20	0.42
1:YA:183:C:H42	1:YA:213:A:H61	1.68	0.42
1:YA:2081:C:H2'	1:YA:2082:A:C8	2.52	0.42
7:YH:16:SER:O	7:YH:26:VAL:HA	2.20	0.42
8:YI:65:ALA:O	8:YI:69:LYS:N	2.53	0.42
26:Y4:61:ARG:HH21	50:XS:9:VAL:HG11	1.85	0.42
32:XA:7:G:H5'	32:XA:298:A:O4'	2.20	0.42
32:XA:1129:C:H4'	32:XA:1130:A:OP1	2.20	0.42
55:XY:108:GLU:HB3	55:XY:170:GLY:H	1.85	0.42
1:RA:117:G:C6	1:RA:119:A:C6	3.08	0.42
1:RA:185:U:H4'	1:RA:218:A:H4'	2.02	0.42
1:RA:323:G:H1'	1:RA:1205:U:O2	2.20	0.42
1:RA:792:G:H5''	1:RA:793:A:H5'	2.01	0.42
1:RA:1087:G:H1	1:RA:1102:C:H42	1.68	0.42
1:RA:2119:A:O2'	1:RA:2120:G:H5'	2.20	0.42
1:RA:2393:A:H2'	1:RA:2394:C:O4'	2.20	0.42
1:RA:2693:A:H2'	1:RA:2694:G:H8	1.85	0.42
7:RH:12:PRO:O	7:RH:15:VAL:HG22	2.19	0.42
15:RT:51:ARG:HG3	15:RT:98:LYS:HE3	2.01	0.42
26:R4:59:PHE:CD1	50:QS:64:GLU:HG3	2.54	0.42
32:QA:1479:C:H2'	32:QA:1480:G:C8	2.55	0.42
33:QB:8:LYS:H	33:QB:8:LYS:HG3	1.60	0.42
33:QB:45:GLN:O	33:QB:49:GLU:HG2	2.19	0.42
33:QB:185:ILE:HG22	33:QB:199:TYR:CD2	2.55	0.42
33:QB:212:GLN:O	33:QB:216:SER:OG	2.37	0.42
34:QC:179:ARG:NH1	34:QC:206:GLU:OE1	2.53	0.42
37:QF:76:ALA:O	37:QF:80:ARG:HG3	2.20	0.42
43:QL:109:GLY:HA3	43:QL:121:GLY:O	2.20	0.42
1:YA:1709:U:H2'	1:YA:1710:C:C6	2.55	0.42
3:YD:69:ARG:HG2	3:YD:130:ALA:HB3	2.02	0.42
6:YG:139:LEU:HA	6:YG:144:ILE:HB	2.02	0.42
7:YH:144:VAL:O	7:YH:148:ILE:HG12	2.20	0.42
10:YO:9:GLU:O	10:YO:83:ALA:HA	2.20	0.42
12:YQ:41:TRP:CD1	12:YQ:96:VAL:HG22	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:YR:96:ARG:HG2	13:YR:115:GLU:HG3	2.01	0.42
14:YS:83:LYS:HB3	14:YS:111:GLU:OE1	2.19	0.42
15:YT:16:ARG:HG2	15:YT:18:ASP:OD1	2.20	0.42
31:Y9:27:CYS:SG	31:Y9:28:GLU:N	2.93	0.42
32:XA:371:G:O2'	32:XA:373:A:N7	2.51	0.42
32:XA:781:A:H4'	32:XA:1522:U:O2'	2.19	0.42
32:XA:865:A:H5'	32:XA:1078:U:C5	2.55	0.42
33:XB:57:PHE:CE2	33:XB:185:ILE:HD11	2.54	0.42
55:XY:310:TYR:HB3	55:XY:329:LEU:HD11	2.02	0.42
1:RA:42:G:H1'	1:RA:437:G:N2	2.35	0.41
1:RA:468:G:H5''	5:RF:60:SER:HB2	2.01	0.41
1:RA:1058:G:N2	1:RA:1080:C:N3	2.61	0.41
1:RA:1356:G:N2	1:RA:1376:C:C2	2.88	0.41
1:RA:1412:A:H2'	1:RA:1413:G:O4'	2.20	0.41
1:RA:1812:A:O2'	3:RD:45:ASN:N	2.52	0.41
1:RA:2061:G:C2	1:RA:2063:C:C4	3.08	0.41
4:RE:94:GLU:OE2	4:RE:177:PRO:HB3	2.20	0.41
18:RW:46:PHE:O	18:RW:50:VAL:HG23	2.20	0.41
19:RX:41:ASN:O	19:RX:45:THR:HG23	2.20	0.41
32:QA:757:U:O2'	32:QA:879:C:O2	2.32	0.41
32:QA:821:G:H2'	32:QA:822:C:C6	2.55	0.41
32:QA:921:U:O2	36:QE:19:MET:HB2	2.19	0.41
32:QA:1323:G:H2'	32:QA:1324:A:C8	2.55	0.41
32:QA:1327:C:H2'	32:QA:1328:C:C6	2.55	0.41
39:QH:119:LEU:HB3	39:QH:123:GLU:HB2	2.01	0.41
41:QJ:35:SER:N	41:QJ:73:ASP:O	2.44	0.41
55:QY:248:HIS:CE1	55:QY:250:PRO:HG2	2.55	0.41
1:YA:272(O):C:H2'	1:YA:272(P):C:C6	2.55	0.41
1:YA:674:G:O2'	5:YF:74:ARG:HD3	2.19	0.41
1:YA:1913:A:OP1	55:XY:160:LYS:HE2	2.20	0.41
1:YA:2286:A:OP1	28:Y6:29:ASN:HB3	2.20	0.41
1:YA:2319:G:H22	14:YS:3:ARG:CZ	2.33	0.41
2:YB:13:A:O2'	2:YB:14:U:H3'	2.19	0.41
5:YF:89:VAL:HG12	5:YF:90:PHE:CD2	2.55	0.41
7:YH:98:LEU:HD12	7:YH:98:LEU:HA	1.86	0.41
32:XA:921:U:H2'	32:XA:922:G:O4'	2.20	0.41
32:XA:1070:U:H2'	32:XA:1071:C:C6	2.55	0.41
42:XK:84:VAL:HG21	42:XK:95:ILE:HD11	2.01	0.41
45:YN:58:LYS:HE3	45:YN:58:LYS:HB3	1.82	0.41
1:RA:738:G:C6	1:RA:739:G:C2	3.08	0.41
1:RA:911:A:H2'	12:RQ:9:TYR:OH	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:RA:1070:A:H2'	1:RA:1071:G:C8	2.55	0.41
1:RA:1080:C:H2'	1:RA:1081:U:C6	2.54	0.41
38:QG:12:LEU:H	38:QG:12:LEU:HD12	1.85	0.41
55:QY:317:VAL:HG23	55:QY:329:LEU:HB2	2.03	0.41
1:YA:272(P):C:O2'	8:YI:42:SER:OG	2.17	0.41
1:YA:434:U:H1'	1:YA:435:C:H5	1.85	0.41
1:YA:671:C:H2'	1:YA:672:C:C6	2.55	0.41
1:YA:2493:U:HO2'	55:XY:264:HIS:CD2	2.38	0.41
28:Y6:6:ARG:NH1	28:Y6:26:ASN:HB2	2.35	0.41
32:XA:176:C:H2'	32:XA:177:C:H6	1.85	0.41
32:XA:324:G:N1	32:XA:327:A:OP2	2.52	0.41
32:XA:1286:A:C8	32:XA:1287:A:H4'	2.55	0.41
32:XA:1346:A:N1	32:XA:1374:A:H5''	2.34	0.41
32:XA:1516:G:H2'	32:XA:1518:MA6:OP2	2.20	0.41
33:XB:19:HIS:CG	33:XB:20:GLU:N	2.88	0.41
40:XI:5:TYR:HE1	40:XI:16:ARG:HB3	1.85	0.41
40:XI:100:GLY:O	40:XI:103:THR:HG22	2.20	0.41
41:XJ:9:ARG:NH2	41:XJ:95:GLU:OE1	2.45	0.41
1:RA:908:C:OP1	12:RQ:22:LYS:HB3	2.20	0.41
1:RA:1213:A:N3	1:RA:1238:G:H1'	2.34	0.41
1:RA:1803:A:H4'	3:RD:259:THR:HG23	2.01	0.41
4:RE:144:ARG:HB3	4:RE:145:LYS:H	1.66	0.41
6:RG:45:GLU:H	6:RG:45:GLU:HG2	1.53	0.41
17:RV:14:VAL:HB	17:RV:96:ILE:HG13	2.02	0.41
17:RV:40:LEU:HB2	17:RV:46:VAL:CG1	2.51	0.41
18:RW:23:LEU:HD11	27:R5:25:LEU:HB2	2.02	0.41
22:R0:27:GLU:HB2	22:R0:69:PHE:HD1	1.85	0.41
24:R2:3:LEU:HD23	24:R2:3:LEU:HA	1.90	0.41
32:QA:1179:A:H2'	32:QA:1180:A:O4'	2.20	0.41
32:QA:1182:G:H5'	32:QA:1184:G:H5'	2.03	0.41
33:QB:15:VAL:O	33:QB:15:VAL:HG22	2.20	0.41
33:QB:146:GLN:O	33:QB:150:SER:HB3	2.20	0.41
36:QE:31:LEU:HD11	36:QE:129:ILE:HA	2.02	0.41
47:QP:34:GLU:OE2	47:QP:55:ARG:NH2	2.54	0.41
47:QP:74:LEU:HB3	47:QP:79:VAL:CG2	2.51	0.41
1:YA:459:U:H2'	1:YA:460:A:C8	2.55	0.41
1:YA:601:C:O2'	1:YA:605:C:H5''	2.21	0.41
1:YA:738:G:C6	1:YA:739:G:C2	3.09	0.41
1:YA:960:A:H2'	1:YA:962:G:H5'	2.02	0.41
1:YA:981:A:HO2'	1:YA:2036:C:HO2'	1.69	0.41
1:YA:1721:G:H2'	1:YA:1740:G:O6	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:YA:1932:A:H2'	1:YA:1933:G:O4'	2.18	0.41
1:YA:2251:OMG:H1'	1:YA:2251:OMG:HM23	1.85	0.41
1:YA:2262:U:OP1	1:YA:2387:U:O2'	2.28	0.41
12:YQ:31:ASP:OD1	12:YQ:134:ARG:NH1	2.44	0.41
23:Y1:82:LEU:O	23:Y1:85:LEU:HD13	2.20	0.41
31:Y9:22:ARG:HB2	31:Y9:24:TYR:CE1	2.55	0.41
32:XA:841:U:OP1	32:XA:841:U:H6	2.03	0.41
32:XA:913:A:H4'	32:XA:914:A:O5'	2.21	0.41
32:XA:1521:G:H2'	32:XA:1522:U:C6	2.54	0.41
38:XG:113:GLU:HG3	38:XG:118:VAL:HG12	2.03	0.41
40:XI:5:TYR:OH	40:XI:16:ARG:HG2	2.20	0.41
45:YN:23:ARG:NH1	45:YN:28:GLY:O	2.50	0.41
48:XQ:4:LYS:H	48:XQ:61:GLU:HG2	1.84	0.41
55:XY:259:ASP:OD1	55:XY:259:ASP:N	2.51	0.41
1:RA:1006:C:O2'	9:RN:106:MET:HB3	2.20	0.41
1:RA:1778:U:H2'	1:RA:1784:A:N6	2.35	0.41
1:RA:1794:U:H2'	1:RA:1795:C:C6	2.56	0.41
1:RA:2679:A:C2	1:RA:2729:G:C2	3.08	0.41
1:RA:2730:C:O2'	4:RE:168:MET:O	2.28	0.41
3:RD:69:ARG:HE	3:RD:130:ALA:HB2	1.86	0.41
5:RF:22:ALA:HB1	5:RF:203:GLN:HE22	1.85	0.41
9:RN:108:PRO:O	9:RN:113:GLY:HA3	2.20	0.41
26:R4:10:VAL:HG21	26:R4:29:PRO:HG3	2.01	0.41
26:R4:50:VAL:HG21	44:QM:64:TRP:C	2.41	0.41
32:QA:159:G:O2'	32:QA:161:A:N7	2.50	0.41
32:QA:1398:A:H5'	32:QA:1401:G:H4'	2.03	0.41
32:QA:1513:A:H2'	32:QA:1514:C:C6	2.55	0.41
35:QD:18:LYS:NZ	35:QD:31:CYS:SG	2.91	0.41
49:QR:65:ILE:O	49:QR:69:THR:HG23	2.21	0.41
1:YA:242:G:O2'	1:YA:254:G:O6	2.29	0.41
1:YA:1654:A:O2'	4:YE:113:PHE:O	2.26	0.41
1:YA:1683:C:H2'	1:YA:1684:C:C6	2.56	0.41
1:YA:1912:A:H4'	55:XY:160:LYS:HZ3	1.85	0.41
3:YD:38:LYS:HA	3:YD:38:LYS:HD2	1.88	0.41
11:YP:126:VAL:HG22	11:YP:146:VAL:HB	2.03	0.41
31:Y9:22:ARG:HB2	31:Y9:24:TYR:HE1	1.84	0.41
32:XA:321:A:H2	32:XA:332:G:H22	1.69	0.41
39:XH:73:ASP:OD1	39:XH:75:ARG:HG3	2.21	0.41
39:XH:85:ARG:NH2	39:XH:87:SER:O	2.53	0.41
39:XH:121:ASP:OD1	39:XH:121:ASP:N	2.51	0.41
44:XM:108:ARG:HA	44:XM:108:ARG:HD3	1.90	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:XR:41:LYS:O	49:XR:41:LYS:HG2	2.20	0.41
51:XT:42:GLN:NE2	51:XT:46:GLU:OE2	2.53	0.41
1:RA:272(M):G:N2	8:RI:50:ARG:HD3	2.35	0.41
1:RA:300:A:H1'	1:RA:319:C:H1'	2.03	0.41
1:RA:304:G:C2	1:RA:305:U:C2	3.09	0.41
1:RA:674:G:C1'	5:RF:74:ARG:HD3	2.50	0.41
1:RA:1789:A:H5'	3:RD:221:VAL:HG12	2.01	0.41
1:RA:2699:C:H2'	1:RA:2700:C:O4'	2.19	0.41
3:RD:106:ILE:O	3:RD:108:PRO:HD3	2.20	0.41
4:RE:47:VAL:HG23	4:RE:84:PHE:O	2.20	0.41
10:RO:22:ILE:HG12	10:RO:40:VAL:O	2.20	0.41
10:RO:73:ASP:HB2	15:RT:82:LEU:HD13	2.03	0.41
17:RV:71:LEU:HD23	17:RV:71:LEU:HA	1.91	0.41
19:RX:56:THR:HB	19:RX:77:LYS:HE3	2.02	0.41
32:QA:345:C:H4'	32:QA:346:G:C4	2.56	0.41
32:QA:437:U:H5'	35:QD:155:LEU:HD21	2.02	0.41
32:QA:689:C:OP1	42:QK:44:SER:OG	2.23	0.41
32:QA:782:A:O3'	32:QA:1515:C:H4'	2.20	0.41
32:QA:1010:G:N2	32:QA:1020:U:H1'	2.35	0.41
33:QB:91:PRO:HG2	33:QB:155:LEU:HD23	2.02	0.41
34:QC:125:GLU:HG3	34:QC:189:ALA:HB1	2.03	0.41
47:QP:79:VAL:HG23	47:QP:80:PHE:CD1	2.55	0.41
1:YA:859:G:O2'	1:YA:916:G:O6	2.35	0.41
1:YA:1900:A:N1	1:YA:1970:A:C6	2.88	0.41
10:YO:4:PRO:HA	10:YO:21:CYS:O	2.20	0.41
11:YP:39:LYS:HD2	11:YP:45:LEU:HD11	2.01	0.41
15:YT:91:ARG:HD2	15:YT:120:ARG:NH1	2.35	0.41
34:XC:28:GLN:HB3	34:XC:32:LEU:HD23	2.02	0.41
35:XD:76:ARG:HD3	35:XD:207:TYR:CE1	2.55	0.41
46:XO:4:THR:CG2	46:XO:7:GLU:H	2.33	0.41
53:XV:47:U:H3'	53:XV:48:C:C5'	2.50	0.41
1:RA:242:G:C8	30:R8:5:LYS:HG2	2.56	0.41
1:RA:675:A:C6	1:RA:676:A:C6	3.08	0.41
5:RF:153:SER:OG	5:RF:190:GLU:HG3	2.20	0.41
14:RS:59:LYS:CD	14:RS:60:GLY:H	2.21	0.41
15:RT:16:ARG:HG2	15:RT:18:ASP:OD1	2.19	0.41
24:R2:63:VAL:HA	24:R2:66:GLU:HB2	2.02	0.41
32:QA:266:G:O3'	48:QQ:67:LYS:HB2	2.19	0.41
32:QA:627:G:H2'	32:QA:628:G:C8	2.55	0.41
32:QA:736:C:H2'	32:QA:737:A:C8	2.56	0.41
35:QD:111:ALA:HB2	35:QD:120:LEU:HD12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:QY:99:LEU:HD12	55:QY:349:GLN:HE22	1.86	0.41
55:QY:221:ASP:HB3	55:QY:250:PRO:CD	2.50	0.41
1:YA:581:C:H2'	1:YA:582:G:C8	2.55	0.41
1:YA:582:G:H2'	1:YA:583:G:C8	2.56	0.41
1:YA:1069:A:H5'	1:YA:1096:A:C5'	2.51	0.41
1:YA:1069:A:H5'	1:YA:1096:A:H5'	2.03	0.41
1:YA:1130:U:C2	4:YE:147:PRO:HB3	2.54	0.41
1:YA:1316:U:H2'	1:YA:1317:A:H8	1.86	0.41
1:YA:1430:C:H2'	1:YA:1431:U:C6	2.55	0.41
1:YA:2361:A:H5'	30:Y8:26:LYS:HZ1	1.84	0.41
2:YB:105:A:H2'	2:YB:106:G:O4'	2.21	0.41
4:YE:116:VAL:HG13	4:YE:122:PHE:HB2	2.02	0.41
23:Y1:77:ALA:O	23:Y1:80:LEU:HB2	2.20	0.41
32:XA:881:G:OP2	43:XL:12:ARG:NH2	2.51	0.41
32:XA:1323:G:H2'	32:XA:1324:A:C8	2.56	0.41
34:XC:180:ALA:HB1	34:XC:203:PHE:CE1	2.55	0.41
41:XJ:7:LYS:HB2	41:XJ:97:GLU:HB2	2.03	0.41
1:RA:309:G:C5	1:RA:330:A:C6	3.09	0.41
1:RA:321:G:H5'	5:RF:134:GLY:O	2.19	0.41
1:RA:1133:U:O4	1:RA:2026:C:H1'	2.21	0.41
1:RA:1899:G:H2'	1:RA:1899:G:N3	2.35	0.41
1:RA:2445:G:OP1	5:RF:74:ARG:NH2	2.53	0.41
4:RE:119:ARG:HG3	4:RE:160:TYR:CG	2.55	0.41
5:RF:110:LEU:HA	5:RF:183:VAL:HG12	2.03	0.41
13:RR:54:LEU:HD12	13:RR:54:LEU:HA	1.97	0.41
21:RZ:103:ARG:HD2	21:RZ:136:PHE:CG	2.56	0.41
32:QA:499:A:H4'	32:QA:500:G:H5'	2.03	0.41
32:QA:619:U:N3	35:QD:134:ASP:OD1	2.38	0.41
32:QA:1143:G:H2'	32:QA:1144:G:H8	1.85	0.41
35:QD:173:TRP:CG	35:QD:189:PRO:HG3	2.55	0.41
35:QD:188:LEU:HD23	35:QD:188:LEU:H	1.85	0.41
37:QF:91:VAL:HG11	49:QR:72:ARG:NH1	2.36	0.41
40:QI:17:VAL:HG23	40:QI:63:ILE:HG12	2.01	0.41
41:QJ:19:SER:O	41:QJ:23:ILE:HG12	2.21	0.41
41:QJ:49:VAL:HG21	45:QN:41:ARG:O	2.21	0.41
45:QN:41:ARG:HG3	45:QN:42:ILE:HG13	2.03	0.41
53:QV:10:G:N2	53:QV:26:G:H1'	2.36	0.41
55:QY:244:ILE:H	55:QY:266:ASN:HD22	1.68	0.41
1:YA:57:C:H2'	1:YA:58:G:O4'	2.21	0.41
1:YA:635:C:O2'	1:YA:639:U:OP1	2.30	0.41
1:YA:687:C:H2'	1:YA:688:U:O4'	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:YA:910:A:N1	1:YA:2277:G:H1'	2.36	0.41
1:YA:2137:C:C2	1:YA:2154:G:N1	2.89	0.41
1:YA:2264:C:H2'	1:YA:2265:U:C6	2.55	0.41
4:YE:12:THR:HG22	4:YE:13:ARG:N	2.32	0.41
4:YE:174:ASP:OD1	4:YE:175:VAL:N	2.54	0.41
9:YN:62:VAL:CG1	9:YN:66:LYS:HB2	2.50	0.41
16:YU:27:LEU:HB3	16:YU:31:SER:HB3	2.03	0.41
18:YW:8:ARG:HG2	18:YW:102:HIS:ND1	2.36	0.41
32:XA:8:A:H5'	36:XE:101:ILE:HG22	2.01	0.41
32:XA:255:G:H2'	32:XA:256:U:C6	2.56	0.41
32:XA:292:G:C5	32:XA:293:G:H1'	2.56	0.41
32:XA:407:G:OP1	35:XD:115:ARG:HD3	2.20	0.41
32:XA:1329:A:P	44:XM:28:ALA:HB3	2.60	0.41
33:XB:24:TRP:CZ3	33:XB:26:PRO:HA	2.55	0.41
35:XD:88:VAL:HG22	36:XE:96:PRO:HB2	2.02	0.41
55:XY:255:VAL:CG1	55:XY:274:LEU:HG	2.45	0.41
1:RA:329:G:H8	1:RA:329:G:P	2.43	0.41
1:RA:523:C:O2	1:RA:554:U:O2'	2.35	0.41
1:RA:559:G:H22	16:RU:49:HIS:CE1	2.39	0.41
1:RA:777:A:H2'	1:RA:778:G:C8	2.56	0.41
1:RA:1073:A:H4'	1:RA:1074:G:OP1	2.21	0.41
1:RA:1092:C:OP2	1:RA:1092:C:H6	2.04	0.41
1:RA:1359:A:H61	1:RA:1372:U:H3	1.69	0.41
1:RA:1421:G:C2	1:RA:1422:G:C8	3.09	0.41
1:RA:2228:G:OP1	3:RD:261:LYS:NZ	2.36	0.41
2:RB:13:A:N1	2:RB:69:G:O2'	2.39	0.41
31:R9:32:HIS:O	31:R9:34:GLN:HG3	2.21	0.41
32:QA:408:A:H2'	32:QA:409:G:O4'	2.21	0.41
32:QA:1418:A:N6	32:QA:1482:G:O2'	2.47	0.41
33:QB:77:ALA:HB2	33:QB:211:ILE:HD13	2.03	0.41
35:QD:108:LEU:HB3	35:QD:110:PHE:CD1	2.56	0.41
1:YA:560:C:H4'	16:YU:52:ARG:HE	1.86	0.41
1:YA:839:U:H2'	1:YA:840:C:C6	2.56	0.41
1:YA:2318:G:N2	14:YS:3:ARG:HH11	2.18	0.41
7:YH:171:LEU:HD23	7:YH:171:LEU:H	1.85	0.41
10:YO:8:LEU:HD12	10:YO:84:ALA:HB2	2.02	0.41
14:YS:43:GLU:OE1	22:Y0:49:LYS:HE3	2.21	0.41
32:XA:189(M):G:H2'	32:XA:190:U:H6	1.86	0.41
32:XA:575:G:O2'	32:XA:821:G:H5'	2.20	0.41
32:XA:738:C:OP1	37:XF:2:ARG:NH1	2.51	0.41
32:XA:979:C:H42	45:YN:18:VAL:HG12	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:XA:1366:C:H2'	32:XA:1367:C:C6	2.55	0.41
35:XD:190:ASP:O	35:XD:193:ASP:HB2	2.20	0.41
36:XE:141:GLN:HA	36:XE:143:ARG:HH21	1.86	0.41
37:XF:100:ASN:HB2	49:XR:27:GLY:O	2.20	0.41
41:XJ:70:ARG:HA	41:XJ:70:ARG:HD3	1.92	0.41
55:XY:129:GLY:HA2	55:XY:159:TYR:HD2	1.86	0.41
1:RA:116:C:H2'	1:RA:117:G:O4'	2.21	0.41
1:RA:337:C:H2'	1:RA:338:G:O4'	2.21	0.41
1:RA:812:C:HO2'	1:RA:1226:A:HO2'	1.62	0.41
1:RA:1055:G:H21	1:RA:1084:A:N6	2.19	0.41
1:RA:1071:G:OP1	1:RA:1073:A:N6	2.53	0.41
1:RA:1482:G:C6	1:RA:1507:A:C6	3.08	0.41
1:RA:1649:G:O2'	13:RR:107:ASP:OD2	2.33	0.41
1:RA:2046:G:H5'	27:R5:19:ARG:HB2	2.03	0.41
1:RA:2070:G:H2'	1:RA:2071:A:O4'	2.21	0.41
1:RA:2122:U:H2'	1:RA:2123:G:C8	2.56	0.41
1:RA:2158:A:H1'	1:RA:2159:G:C8	2.56	0.41
1:RA:2306:C:C4	1:RA:2307:G:C6	3.08	0.41
4:RE:143:ASN:HD22	4:RE:147:PRO:CD	2.34	0.41
6:RG:53:LEU:H	6:RG:53:LEU:HD23	1.86	0.41
7:RH:98:LEU:HD12	7:RH:98:LEU:HA	1.97	0.41
10:RO:80:ASP:OD1	15:RT:64:ARG:NH2	2.54	0.41
12:RQ:35:VAL:HG13	12:RQ:130:LYS:HB3	2.03	0.41
16:RU:28:ARG:NH1	16:RU:38:THR:OG1	2.47	0.41
21:RZ:198:LYS:HE2	53:QV:52:G:H2'	2.02	0.41
32:QA:7:G:O2'	36:QE:120:THR:O	2.39	0.41
32:QA:58:C:O2'	32:QA:388:G:N7	2.50	0.41
32:QA:193:C:H4'	51:QT:60:GLU:HG2	2.03	0.41
32:QA:266:G:H5''	32:QA:267:C:C5	2.56	0.41
32:QA:540:G:H2'	32:QA:541:G:O4'	2.21	0.41
32:QA:1005:A:OP1	32:QA:1006:C:N4	2.53	0.41
32:QA:1441:G:H4'	32:QA:1442(A):G:C4	2.56	0.41
32:QA:1466:C:H2'	32:QA:1467:G:O4'	2.21	0.41
34:QC:6:HIS:HE1	34:QC:8:ILE:HB	1.83	0.41
35:QD:8:VAL:HG22	35:QD:21:LEU:HD13	2.03	0.41
35:QD:188:LEU:HA	35:QD:189:PRO:HD3	1.91	0.41
37:QF:41:GLU:HG2	37:QF:43:LEU:HD12	2.02	0.41
41:QJ:78:ASN:O	41:QJ:80:LYS:N	2.54	0.41
41:QJ:84:GLN:HE21	41:QJ:84:GLN:HB3	1.61	0.41
55:QY:214:LEU:HD12	55:QY:215:PRO:CD	2.50	0.41
1:YA:646:A:H2'	1:YA:647:G:O4'	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:YA:1420:U:O2'	1:YA:1421:G:OP1	2.31	0.41
1:YA:1472:A:H2'	1:YA:1473:G:O4'	2.21	0.41
1:YA:2031:A:N3	1:YA:2455:G:O2'	2.49	0.41
1:YA:2287:A:C8	1:YA:2289:G:C8	3.08	0.41
1:YA:2405:G:H5'	11:YP:75:ILE:HD13	2.03	0.41
2:YB:12:C:H2'	22:Y0:73:GLY:HA3	2.03	0.41
4:YE:179:GLU:HG3	15:YT:9:LEU:CD2	2.51	0.41
5:YF:11:VAL:HG22	5:YF:125:LEU:HB2	2.03	0.41
9:YN:35:ARG:HH21	9:YN:42:TRP:HZ2	1.68	0.41
12:YQ:137:TYR:O	12:YQ:141:GLN:HG2	2.21	0.41
14:YS:11:LYS:HG3	14:YS:91:PRO:HD3	2.02	0.41
16:YU:36:ARG:HD3	16:YU:40:PHE:CZ	2.56	0.41
20:YY:13:VAL:O	20:YY:24:VAL:HA	2.21	0.41
32:XA:20:U:H2'	32:XA:21:G:O4'	2.20	0.41
32:XA:449:C:O2	47:XP:42:ARG:HD2	2.21	0.41
32:XA:663:A:H5''	49:XR:61:LYS:NZ	2.36	0.41
32:XA:728:A:C8	46:XO:54:ARG:NH2	2.88	0.41
32:XA:796:C:O5'	32:XA:796:C:H6	2.03	0.41
32:XA:952:U:H2'	32:XA:953:G:C8	2.56	0.41
32:XA:1070:U:H2'	32:XA:1071:C:H6	1.85	0.41
32:XA:1099:G:OP2	33:XB:144:ARG:NH2	2.54	0.41
32:XA:1225:A:H2'	32:XA:1226:C:C5	2.56	0.41
32:XA:1518:MA6:H93	32:XA:1519:MA6:N6	2.36	0.41
34:XC:50:ALA:HB1	34:XC:70:VAL:HG21	2.03	0.41
36:XE:78:HIS:CG	39:XH:104:ARG:HD2	2.56	0.41
39:XH:96:GLY:N	39:XH:99:GLU:HG3	2.36	0.41
44:XM:22:ILE:HB	44:XM:25:ILE:HD12	2.03	0.41
47:XP:4:ILE:HG23	47:XP:36:ILE:HD11	2.03	0.41
47:XP:20:VAL:HG23	47:XP:35:LYS:HA	2.03	0.41
55:XY:183:ARG:O	55:XY:309:THR:HA	2.20	0.41
1:RA:392:C:H5''	1:RA:409:C:H5''	2.02	0.41
1:RA:411:G:C5	11:RP:72:PRO:HB3	2.56	0.41
1:RA:500:G:N1	1:RA:503:A:OP2	2.54	0.41
1:RA:859:G:O2'	1:RA:916:G:O6	2.35	0.41
1:RA:1053:C:H4'	1:RA:1054:A:OP1	2.21	0.41
1:RA:2075:U:C4	1:RA:2238:G:C6	3.08	0.41
1:RA:2391:G:O6	1:RA:2425:A:H8	2.03	0.41
1:RA:2502:G:H5''	1:RA:2503:2MA:H5''	2.03	0.41
1:RA:2503:2MA:H4'	1:RA:2504:U:OP1	2.21	0.41
1:RA:2507:C:C2	1:RA:2508:G:C8	3.09	0.41
1:RA:2578:G:OP1	1:RA:2614:A:N6	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:RA:2717:G:H1'	15:RT:96:ARG:HH21	1.86	0.41
1:RA:2849:U:H4'	1:RA:2868:A:C2	2.56	0.41
7:RH:69:ARG:HH11	7:RH:69:ARG:HD3	1.62	0.41
11:RP:88:LEU:HD11	11:RP:114:ILE:HD12	2.02	0.41
32:QA:36:C:OP1	43:QL:123:LYS:HE2	2.21	0.41
32:QA:255:G:C2	32:QA:272:C:C2	3.09	0.41
32:QA:441:A:H3'	32:QA:442:C:H6	1.86	0.41
32:QA:757:U:H2'	32:QA:758:G:O4'	2.21	0.41
32:QA:772:U:C4	32:QA:773:G:N7	2.89	0.41
32:QA:1492:A:O2'	55:QY:119:THR:HG23	2.20	0.41
34:QC:5:ILE:HD13	41:QJ:51:ARG:HH12	1.86	0.41
34:QC:58:GLU:CB	41:QJ:92:THR:HG21	2.49	0.41
40:QI:8:GLY:HA3	40:QI:76:ALA:O	2.21	0.41
41:QJ:21:GLN:O	41:QJ:25:GLU:HG3	2.20	0.41
53:QV:19:G:H5'	53:QV:20:U:H5	1.86	0.41
1:YA:613:G:O2'	1:YA:614(D):A:N1	2.40	0.41
1:YA:775:G:C4	1:YA:794:G:C8	3.09	0.41
1:YA:1317:A:H2'	1:YA:1318:C:C6	2.56	0.41
1:YA:2077:A:H2'	1:YA:2078:C:H6	1.86	0.41
1:YA:2330:G:H2'	1:YA:2331:G:O4'	2.21	0.41
1:YA:2359:C:H2'	1:YA:2360:A:O4'	2.20	0.41
1:YA:2680:C:H5'	4:YE:189:PRO:HA	2.02	0.41
1:YA:2887:U:H2'	1:YA:2888:C:C6	2.55	0.41
7:YH:140:LYS:HE3	7:YH:140:LYS:HB2	1.89	0.41
9:YN:120:LEU:HD22	9:YN:122:VAL:HG23	2.03	0.41
10:YO:105:GLU:OE1	10:YO:105:GLU:N	2.49	0.41
12:YQ:29:PHE:O	21:YZ:122:ARG:NH2	2.52	0.41
20:YY:35:TYR:CE2	20:YY:69:ALA:HB3	2.56	0.41
21:YZ:72:ARG:HH11	21:YZ:72:ARG:HD2	1.75	0.41
24:Y2:12:GLU:HA	24:Y2:15:LYS:NZ	2.36	0.41
25:Y3:26:LEU:O	25:Y3:35:ARG:NE	2.48	0.41
26:Y4:61:ARG:HG2	50:XS:42:PRO:CG	2.51	0.41
32:XA:25:C:H2'	32:XA:26:A:C8	2.55	0.41
32:XA:530:G:C6	54:XX:21:A:C4	3.08	0.41
32:XA:539:A:H2'	32:XA:540:G:H8	1.84	0.41
32:XA:946:A:H2'	32:XA:947:G:C8	2.55	0.41
36:XE:69:VAL:HA	36:XE:70:PRO:HD3	1.84	0.41
40:XI:121:ARG:NH1	40:XI:122:ALA:O	2.53	0.41
55:XY:328:ARG:NH1	55:XY:331:GLU:OE1	2.42	0.41
1:RA:241:A:H8	1:RA:241:A:OP1	2.04	0.40
1:RA:674:G:O2'	5:RF:74:ARG:HD3	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:RA:2577:A:H2'	1:RA:2614:A:N6	2.36	0.40
16:RU:86:ALA:O	17:RV:49:THR:HG23	2.21	0.40
19:RX:60:ARG:NH1	29:R7:47:ARG:HH12	2.19	0.40
20:RY:56:PRO:C	20:RY:58:GLY:H	2.25	0.40
21:RZ:28:MET:HG3	21:RZ:90:VAL:CG2	2.51	0.40
32:QA:31:G:N7	32:QA:306:G:H1'	2.36	0.40
32:QA:652:U:O4	32:QA:752:G:O2'	2.29	0.40
32:QA:1005:A:H8	32:QA:1005:A:O5'	2.04	0.40
34:QC:181:ASN:OD1	34:QC:204:LEU:HD12	2.20	0.40
35:QD:111:ALA:HB1	35:QD:116:GLN:HB3	2.03	0.40
42:QK:78:GLN:O	42:QK:103:LEU:HD23	2.22	0.40
49:QR:28:GLU:H	49:QR:28:GLU:HG2	1.63	0.40
55:QY:322:ILE:HD11	55:QY:344:ILE:HA	2.03	0.40
1:YA:588:U:H1'	5:YF:90:PHE:HB3	2.02	0.40
1:YA:753:C:H2'	1:YA:754:C:H6	1.86	0.40
1:YA:947:G:H2'	1:YA:948:G:C8	2.56	0.40
1:YA:1427:A:H4'	1:YA:1428:C:O4'	2.21	0.40
1:YA:2001:A:H2'	1:YA:2002:G:C8	2.56	0.40
1:YA:2181:G:H2'	1:YA:2182:G:O4'	2.21	0.40
1:YA:2818:G:O2'	1:YA:2819:G:H5'	2.21	0.40
1:YA:2823:A:OP1	4:YE:113:PHE:HB2	2.20	0.40
4:YE:18:ASP:HB3	15:YT:82:LEU:HD21	2.03	0.40
5:YF:53:THR:CG2	5:YF:56:GLU:HG3	2.52	0.40
15:YT:39:ARG:NH1	15:YT:41:ARG:HD3	2.36	0.40
24:Y2:65:ASN:OD1	24:Y2:69:ARG:NH1	2.53	0.40
32:XA:217:C:H2'	32:XA:218:C:C6	2.56	0.40
32:XA:411:A:OP1	35:XD:30:LYS:NZ	2.37	0.40
32:XA:539:A:OP2	43:XL:115:LYS:NZ	2.54	0.40
32:XA:657:G:C2	32:XA:658:G:C8	3.09	0.40
32:XA:687:A:H4'	32:XA:688:G:OP1	2.21	0.40
32:XA:1289:A:N1	32:XA:1371:G:O2'	2.40	0.40
32:XA:1458:G:H5''	51:XT:31:SER:HB2	2.02	0.40
36:XE:92:LYS:HB3	36:XE:119:LEU:HB2	2.03	0.40
44:XM:13:LYS:HA	44:XM:44:ARG:HH11	1.86	0.40
44:XM:57:ARG:O	44:XM:61:GLU:HG3	2.21	0.40
1:RA:37:C:H2'	1:RA:38:A:C8	2.55	0.40
1:RA:1583:A:H5''	1:RA:1584:C:OP1	2.21	0.40
1:RA:2033:A:O2'	1:RA:2035:G:OP2	2.29	0.40
1:RA:2315:G:H2'	1:RA:2316:C:C6	2.56	0.40
1:RA:2519:U:C4	1:RA:2542:A:C5	3.10	0.40
1:RA:2870:C:H5''	13:RR:65:LEU:HD21	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:RB:7:G:H8	2:RB:7:G:H5''	1.86	0.40
2:RB:33:G:C6	2:RB:34:U:C4	3.09	0.40
20:RY:5:MET:HE3	20:RY:32:PRO:HA	2.03	0.40
23:R1:23:LYS:HB3	23:R1:29:GLY:HA3	2.03	0.40
27:R5:35:GLU:HG2	27:R5:51:TYR:CD2	2.56	0.40
32:QA:35:G:O2'	43:QL:118:SER:O	2.28	0.40
32:QA:1277:C:O2'	32:QA:1279:A:H1'	2.20	0.40
32:QA:1280:A:O2'	32:QA:1281:U:H5'	2.21	0.40
1:YA:225:A:O2'	1:YA:257:A:H4'	2.20	0.40
1:YA:272(F):C:H2'	1:YA:272(G):C:C6	2.56	0.40
1:YA:1064:C:H5	1:YA:1065:U:C6	2.38	0.40
1:YA:2018:G:O2'	16:YU:34:LYS:HE3	2.21	0.40
1:YA:2667:C:H2'	1:YA:2668:G:O4'	2.21	0.40
1:YA:2732:G:H3'	1:YA:2733:A:O4'	2.20	0.40
2:YB:77:U:OP1	21:YZ:19:ARG:NH2	2.53	0.40
3:YD:18:VAL:HG12	3:YD:211:ARG:NH1	2.37	0.40
5:YF:192:LEU:HD22	5:YF:194:MET:HG3	2.03	0.40
7:YH:113:VAL:HG11	7:YH:151:ILE:HD13	2.02	0.40
9:YN:99:LEU:HD23	9:YN:99:LEU:HA	1.81	0.40
10:YO:70:LYS:HE2	10:YO:70:LYS:HB3	1.91	0.40
12:YQ:35:VAL:HG12	12:YQ:130:LYS:O	2.21	0.40
32:XA:18:C:H4'	32:XA:1078:U:O2	2.21	0.40
32:XA:163:C:H2'	32:XA:164:U:O4'	2.21	0.40
32:XA:581:G:OP1	46:XO:65:ARG:NH2	2.48	0.40
33:XB:101:MET:HG2	33:XB:108:ILE:HG21	2.02	0.40
49:XR:76:LEU:HD12	49:XR:76:LEU:HA	1.89	0.40
1:RA:321:G:O2'	1:RA:340:A:N3	2.52	0.40
1:RA:820:A:H2'	1:RA:821:A:O4'	2.22	0.40
1:RA:1425:G:H2'	1:RA:1426:G:O4'	2.21	0.40
1:RA:2553:G:C2	1:RA:2583:G:H1'	2.56	0.40
2:RB:105:A:H2'	2:RB:106:G:O4'	2.22	0.40
4:RE:2:LYS:HB2	4:RE:95:ILE:HD12	2.02	0.40
6:RG:50:ALA:C	6:RG:52:ILE:N	2.74	0.40
6:RG:64:THR:HB	6:RG:94:LEU:HD21	2.03	0.40
12:RQ:35:VAL:HG12	12:RQ:130:LYS:O	2.21	0.40
18:RW:14:PRO:HG2	18:RW:78:GLU:HG2	2.02	0.40
21:RZ:35:ARG:HA	21:RZ:35:ARG:HD2	1.93	0.40
32:QA:637:G:H2'	32:QA:638:G:C8	2.56	0.40
33:QB:169:LYS:HG3	33:QB:170:GLU:OE1	2.22	0.40
48:QQ:62:SER:OG	48:QQ:72:ARG:HG3	2.21	0.40
55:QY:105:PRO:C	55:QY:107:ASP:H	2.24	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:YA:249:C:O2	30:Y8:12:LYS:NZ	2.31	0.40
1:YA:612:C:H2'	1:YA:613:G:O4'	2.20	0.40
1:YA:724:U:H2'	1:YA:725:G:O4'	2.21	0.40
1:YA:1359:A:N3	1:YA:1359:A:H5'	2.36	0.40
1:YA:1417:C:H2'	1:YA:1418:G:O4'	2.21	0.40
1:YA:1598:C:H2'	1:YA:1599:C:C6	2.56	0.40
1:YA:1668:A:C8	1:YA:1674:G:C6	3.09	0.40
1:YA:2679:A:H4'	4:YE:165:VAL:HG11	2.02	0.40
2:YB:17:C:H2'	2:YB:18:G:O4'	2.21	0.40
2:YB:75:G:H4'	21:YZ:36:LYS:HG2	2.02	0.40
3:YD:102:LYS:O	3:YD:103:ARG:HG2	2.21	0.40
6:YG:16:ARG:NE	6:YG:31:VAL:HG21	2.34	0.40
12:YQ:75:THR:HA	12:YQ:89:ASN:O	2.21	0.40
16:YU:112:ARG:HG2	16:YU:112:ARG:H	1.73	0.40
21:YZ:92:SER:O	21:YZ:130:PRO:HG2	2.22	0.40
32:XA:986:A:H2'	32:XA:987:G:O4'	2.21	0.40
32:XA:1133:G:H2'	32:XA:1134:G:C8	2.57	0.40
33:XB:41:ILE:HD13	33:XB:41:ILE:HA	1.78	0.40
34:XC:43:LEU:HB3	34:XC:47:LEU:HD12	2.03	0.40
38:XG:114:ARG:HB2	38:XG:115:ARG:HH21	1.86	0.40
47:XP:14:ASN:HD22	47:XP:42:ARG:NH2	2.19	0.40
47:XP:75:ARG:HG3	47:XP:80:PHE:CD2	2.56	0.40
53:XV:52:G:C2	53:XV:63:G:C2	3.10	0.40
53:XV:76:A:H3'	55:XY:234:GLY:HA3	2.03	0.40
55:XY:183:ARG:NH2	55:XY:309:THR:HG21	2.36	0.40
1:RA:272(K):U:H1'	8:RI:50:ARG:NH2	2.36	0.40
1:RA:523:C:H4'	1:RA:540:C:O2	2.20	0.40
5:RF:29:ASN:H	5:RF:112:MET:HE3	1.86	0.40
7:RH:4:ILE:O	7:RH:69:ARG:HG2	2.21	0.40
13:RR:96:ARG:NH1	13:RR:115:GLU:OE1	2.52	0.40
22:R0:22:GLY:N	22:R0:39:ARG:O	2.43	0.40
31:R9:10:ILE:HD12	31:R9:32:HIS:HA	2.02	0.40
32:QA:582:U:OP1	46:QO:64:ARG:NH1	2.55	0.40
32:QA:790:A:C6	32:QA:791:G:C6	3.09	0.40
46:QO:8:LYS:O	46:QO:12:ILE:HG13	2.21	0.40
1:YA:300:A:H1'	1:YA:319:C:H1'	2.04	0.40
1:YA:329:G:H8	1:YA:329:G:P	2.44	0.40
1:YA:1093:G:H2'	1:YA:1094:U:O4'	2.21	0.40
1:YA:1486:A:H2'	1:YA:1487:G:H8	1.86	0.40
1:YA:2314:C:H5'	6:YG:38:VAL:HG11	2.04	0.40
6:YG:43:LEU:HB3	6:YG:44:GLY:H	1.70	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:Y0:19:LYS:HD3	22:Y0:19:LYS:HA	1.86	0.40
32:XA:101:A:H5''	51:XT:10:LEU:HD21	2.03	0.40
32:XA:403:C:OP1	35:XD:137:SER:OG	2.32	0.40
32:XA:542:G:H5'	35:XD:41:GLY:HA3	2.03	0.40
32:XA:1492:A:O4'	43:XL:47:LYS:HD3	2.22	0.40
34:XC:8:ILE:HG12	34:XC:184:TYR:HB3	2.02	0.40
34:XC:140:ARG:NH1	34:XC:140:ARG:HB2	2.36	0.40
37:XF:82:ARG:HB2	37:XF:85:VAL:HG23	2.03	0.40
42:XK:65:ALA:HB3	42:XK:97:ALA:HB3	2.03	0.40
44:XM:16:ASP:OD1	44:XM:16:ASP:N	2.53	0.40
1:RA:536:A:H2'	1:RA:537:C:C6	2.56	0.40
1:RA:643:A:N1	1:RA:2369:A:O2'	2.44	0.40
1:RA:1789:A:OP1	3:RD:221:VAL:HA	2.21	0.40
1:RA:1817:G:C6	1:RA:1818:U:C4	3.10	0.40
1:RA:1907:G:C2	1:RA:1908:C:C2	3.10	0.40
1:RA:2106:G:C6	1:RA:2107:C:C2	3.10	0.40
1:RA:2540:C:H2'	1:RA:2541:A:O4'	2.21	0.40
3:RD:5:LYS:HB3	3:RD:5:LYS:HE3	1.85	0.40
8:RI:61:ARG:HD3	8:RI:61:ARG:HA	1.74	0.40
14:RS:39:ILE:HB	14:RS:49:VAL:HG12	2.03	0.40
30:R8:23:VAL:CG1	30:R8:47:LYS:HB3	2.51	0.40
32:QA:427:U:OP1	35:QD:13:ARG:NH2	2.55	0.40
32:QA:947:G:H2'	32:QA:948:C:O4'	2.21	0.40
32:QA:1279:A:O2'	32:QA:1281:U:OP2	2.22	0.40
36:QE:126:ARG:HG3	36:QE:126:ARG:NH1	2.30	0.40
40:QI:4:TYR:O	40:QI:19:LEU:N	2.40	0.40
55:QY:101:LEU:H	55:QY:102:PRO:HD2	1.87	0.40
55:QY:214:LEU:H	55:QY:215:PRO:HD3	1.85	0.40
1:YA:242:G:C8	30:Y8:3:LYS:HG3	2.56	0.40
1:YA:307:G:N2	1:YA:309:G:H3'	2.37	0.40
4:YE:52:LEU:O	4:YE:76:ARG:N	2.49	0.40
5:YF:130:ALA:HB3	5:YF:142:TRP:HD1	1.87	0.40
14:YS:20:ARG:HD3	14:YS:20:ARG:O	2.21	0.40
16:YU:65:ILE:CD1	16:YU:95:LEU:HB3	2.51	0.40
20:YY:38:ILE:HD11	20:YY:66:PRO:HG3	2.03	0.40
21:YZ:35:ARG:HD2	21:YZ:35:ARG:HA	1.94	0.40
21:YZ:183:LEU:HD23	21:YZ:183:LEU:HA	1.95	0.40
26:Y4:64:GLY:C	26:Y4:66:SER:N	2.75	0.40
32:XA:266:G:O3'	48:XQ:67:LYS:HB2	2.22	0.40
32:XA:404:U:H5''	35:XD:122:ARG:HD3	2.03	0.40
32:XA:936:C:H2'	32:XA:937:A:O4'	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:XA:1273:G:H3'	32:XA:1274:G:H8	1.86	0.40
33:XB:9:GLU:O	33:XB:11:LEU:N	2.55	0.40
37:XF:45:LEU:HD23	37:XF:57:GLN:OE1	2.21	0.40
42:XK:92:GLU:O	42:XK:96:ARG:HD2	2.22	0.40
43:XL:8:ASN:O	43:XL:12:ARG:HG3	2.21	0.40
55:XY:119:THR:O	55:XY:199:SER:HB2	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:R2:46:GLN:OE1	1:YA:277:C:O2'[3_555]	2.02	0.18

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	RD	273/276 (99%)	263 (96%)	10 (4%)	0	100	100
3	YD	273/276 (99%)	262 (96%)	11 (4%)	0	100	100
4	RE	202/206 (98%)	195 (96%)	6 (3%)	1 (0%)	29	65
4	YE	202/206 (98%)	194 (96%)	8 (4%)	0	100	100
5	RF	201/210 (96%)	196 (98%)	5 (2%)	0	100	100
5	YF	201/210 (96%)	194 (96%)	6 (3%)	1 (0%)	29	65
6	RG	179/182 (98%)	168 (94%)	9 (5%)	2 (1%)	14	47
6	YG	179/182 (98%)	169 (94%)	9 (5%)	1 (1%)	25	60
7	RH	172/180 (96%)	164 (95%)	8 (5%)	0	100	100
7	YH	171/180 (95%)	163 (95%)	8 (5%)	0	100	100
8	RI	145/148 (98%)	134 (92%)	10 (7%)	1 (1%)	22	57

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	YI	144/148 (97%)	136 (94%)	8 (6%)	0	100	100
9	RN	138/140 (99%)	134 (97%)	4 (3%)	0	100	100
9	YN	138/140 (99%)	134 (97%)	4 (3%)	0	100	100
10	RO	120/122 (98%)	114 (95%)	6 (5%)	0	100	100
10	YO	120/122 (98%)	113 (94%)	7 (6%)	0	100	100
11	RP	147/150 (98%)	141 (96%)	5 (3%)	1 (1%)	22	57
11	YP	147/150 (98%)	141 (96%)	5 (3%)	1 (1%)	22	57
12	RQ	139/141 (99%)	136 (98%)	3 (2%)	0	100	100
12	YQ	139/141 (99%)	136 (98%)	3 (2%)	0	100	100
13	RR	116/118 (98%)	114 (98%)	2 (2%)	0	100	100
13	YR	116/118 (98%)	112 (97%)	4 (3%)	0	100	100
14	RS	108/112 (96%)	104 (96%)	3 (3%)	1 (1%)	17	52
14	YS	108/112 (96%)	105 (97%)	3 (3%)	0	100	100
15	RT	129/146 (88%)	124 (96%)	5 (4%)	0	100	100
15	YT	129/146 (88%)	125 (97%)	4 (3%)	0	100	100
16	RU	114/118 (97%)	114 (100%)	0	0	100	100
16	YU	114/118 (97%)	113 (99%)	1 (1%)	0	100	100
17	RV	99/101 (98%)	95 (96%)	4 (4%)	0	100	100
17	YV	99/101 (98%)	96 (97%)	2 (2%)	1 (1%)	15	49
18	RW	110/113 (97%)	109 (99%)	1 (1%)	0	100	100
18	YW	110/113 (97%)	109 (99%)	1 (1%)	0	100	100
19	RX	93/96 (97%)	92 (99%)	1 (1%)	0	100	100
19	YX	93/96 (97%)	92 (99%)	0	1 (1%)	14	47
20	RY	105/110 (96%)	98 (93%)	7 (7%)	0	100	100
20	YY	105/110 (96%)	101 (96%)	4 (4%)	0	100	100
21	RZ	201/206 (98%)	196 (98%)	5 (2%)	0	100	100
21	YZ	199/206 (97%)	194 (98%)	5 (2%)	0	100	100
22	R0	75/85 (88%)	73 (97%)	2 (3%)	0	100	100
22	Y0	75/85 (88%)	72 (96%)	3 (4%)	0	100	100
23	R1	95/98 (97%)	94 (99%)	0	1 (1%)	14	47
23	Y1	95/98 (97%)	92 (97%)	2 (2%)	1 (1%)	14	47

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
24	R2	68/72 (94%)	68 (100%)	0	0	100	100
24	Y2	68/72 (94%)	68 (100%)	0	0	100	100
25	R3	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
25	Y3	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
26	R4	67/71 (94%)	55 (82%)	7 (10%)	5 (8%)	1	4
26	Y4	67/71 (94%)	56 (84%)	9 (13%)	2 (3%)	4	21
27	R5	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
27	Y5	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
28	R6	51/54 (94%)	49 (96%)	2 (4%)	0	100	100
28	Y6	51/54 (94%)	49 (96%)	2 (4%)	0	100	100
29	R7	46/49 (94%)	46 (100%)	0	0	100	100
29	Y7	46/49 (94%)	46 (100%)	0	0	100	100
30	R8	62/65 (95%)	62 (100%)	0	0	100	100
30	Y8	62/65 (95%)	62 (100%)	0	0	100	100
31	R9	35/37 (95%)	35 (100%)	0	0	100	100
31	Y9	35/37 (95%)	35 (100%)	0	0	100	100
33	QB	229/256 (90%)	204 (89%)	17 (7%)	8 (4%)	3	18
33	XB	229/256 (90%)	203 (89%)	21 (9%)	5 (2%)	6	28
34	QC	204/239 (85%)	191 (94%)	13 (6%)	0	100	100
34	XC	204/239 (85%)	189 (93%)	14 (7%)	1 (0%)	29	65
35	QD	206/209 (99%)	196 (95%)	10 (5%)	0	100	100
35	XD	206/209 (99%)	199 (97%)	7 (3%)	0	100	100
36	QE	146/162 (90%)	145 (99%)	1 (1%)	0	100	100
36	XE	146/162 (90%)	145 (99%)	1 (1%)	0	100	100
37	QF	98/101 (97%)	96 (98%)	2 (2%)	0	100	100
37	XF	98/101 (97%)	96 (98%)	2 (2%)	0	100	100
38	QG	153/156 (98%)	150 (98%)	3 (2%)	0	100	100
38	XG	153/156 (98%)	150 (98%)	3 (2%)	0	100	100
39	QH	135/138 (98%)	133 (98%)	2 (2%)	0	100	100
39	XH	135/138 (98%)	133 (98%)	2 (2%)	0	100	100
40	QI	125/128 (98%)	116 (93%)	9 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
40	XI	124/128 (97%)	113 (91%)	9 (7%)	2 (2%)	9	37
41	QJ	95/105 (90%)	81 (85%)	11 (12%)	3 (3%)	4	20
41	XJ	94/105 (90%)	83 (88%)	10 (11%)	1 (1%)	14	47
42	QK	112/129 (87%)	105 (94%)	7 (6%)	0	100	100
42	XK	112/129 (87%)	106 (95%)	5 (4%)	1 (1%)	17	52
43	QL	119/132 (90%)	118 (99%)	1 (1%)	0	100	100
43	XL	119/132 (90%)	117 (98%)	2 (2%)	0	100	100
44	QM	114/126 (90%)	105 (92%)	8 (7%)	1 (1%)	17	52
44	XM	112/126 (89%)	104 (93%)	7 (6%)	1 (1%)	17	52
45	QN	58/61 (95%)	56 (97%)	2 (3%)	0	100	100
45	XN	58/61 (95%)	56 (97%)	2 (3%)	0	100	100
46	QO	86/89 (97%)	83 (96%)	3 (4%)	0	100	100
46	XO	86/89 (97%)	82 (95%)	4 (5%)	0	100	100
47	QP	80/88 (91%)	77 (96%)	3 (4%)	0	100	100
47	XP	80/88 (91%)	77 (96%)	3 (4%)	0	100	100
48	QQ	97/105 (92%)	94 (97%)	3 (3%)	0	100	100
48	XQ	97/105 (92%)	95 (98%)	2 (2%)	0	100	100
49	QR	66/88 (75%)	66 (100%)	0	0	100	100
49	XR	66/88 (75%)	66 (100%)	0	0	100	100
50	QS	81/93 (87%)	77 (95%)	4 (5%)	0	100	100
50	XS	81/93 (87%)	77 (95%)	4 (5%)	0	100	100
51	QT	94/106 (89%)	90 (96%)	3 (3%)	1 (1%)	14	47
51	XT	96/106 (91%)	90 (94%)	4 (4%)	2 (2%)	7	30
52	QU	21/27 (78%)	19 (90%)	2 (10%)	0	100	100
52	XU	21/27 (78%)	20 (95%)	1 (5%)	0	100	100
55	QY	257/360 (71%)	218 (85%)	21 (8%)	18 (7%)	1	5
55	XY	258/360 (72%)	215 (83%)	30 (12%)	13 (5%)	2	11
All	All	11955/12848 (93%)	11397 (95%)	481 (4%)	77 (1%)	25	60

All (77) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
26	R4	47	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
26	R4	49	PHE
33	QB	16	HIS
55	QY	98	VAL
55	QY	210	PRO
55	QY	241	ASP
55	QY	304	SER
5	YF	21	ALA
23	Y1	3	LYS
26	Y4	60	GLN
33	XB	17	PHE
40	XI	44	VAL
40	XI	54	ASP
44	XM	67	GLU
51	XT	95	ALA
55	XY	216	ASP
55	XY	241	ASP
6	RG	51	ARG
26	R4	45	GLY
26	R4	55	ARG
33	QB	17	PHE
41	QJ	31	GLY
41	QJ	78	ASN
51	QT	95	ALA
55	QY	211	ASP
55	QY	214	LEU
55	QY	299	GLY
55	QY	324	LEU
55	QY	337	LEU
6	YG	81	LYS
33	XB	20	GLU
33	XB	124	SER
55	XY	106	ASP
55	XY	217	ILE
55	XY	306	ARG
26	R4	57	GLU
55	QY	101	LEU
33	XB	10	LEU
33	XB	125	PRO
41	XJ	78	ASN
55	XY	101	LEU
55	XY	102	PRO
55	XY	324	LEU

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Mol	Chain	Res	Type
4	RE	52	LEU
6	RG	49	ASP
33	QB	21	ARG
55	QY	99	LEU
55	QY	109	ARG
55	QY	213	GLU
33	QB	20	GLU
44	QM	12	ASN
55	QY	143	ARG
55	QY	305	ASP
55	QY	322	ILE
55	XY	305	ASP
55	XY	323	ASN
55	XY	337	LEU
8	RI	73	GLU
23	R1	3	LYS
33	QB	127	ILE
55	QY	217	ILE
26	Y4	55	ARG
34	XC	108	ASN
55	QY	313	PRO
51	XT	100	ILE
33	QB	124	SER
41	QJ	77	PRO
11	YP	122	PRO
17	YV	79	VAL
11	RP	122	PRO
14	RS	60	GLY
33	QB	231	GLU
42	XK	118	GLY
55	XY	301	GLY
19	YX	94	GLY
55	XY	299	GLY
33	QB	125	PRO

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	RD	214/218 (98%)	210 (98%)	4 (2%)	57	82
3	YD	215/218 (99%)	209 (97%)	6 (3%)	43	75
4	RE	164/166 (99%)	157 (96%)	7 (4%)	29	63
4	YE	164/166 (99%)	157 (96%)	7 (4%)	29	63
5	RF	160/166 (96%)	151 (94%)	9 (6%)	21	54
5	YF	159/166 (96%)	153 (96%)	6 (4%)	33	67
6	RG	144/156 (92%)	139 (96%)	5 (4%)	36	69
6	YG	142/156 (91%)	134 (94%)	8 (6%)	21	54
7	RH	144/148 (97%)	141 (98%)	3 (2%)	53	80
7	YH	143/148 (97%)	138 (96%)	5 (4%)	36	69
8	RI	111/124 (90%)	106 (96%)	5 (4%)	27	62
8	YI	108/124 (87%)	99 (92%)	9 (8%)	11	37
9	RN	119/119 (100%)	113 (95%)	6 (5%)	24	58
9	YN	118/119 (99%)	111 (94%)	7 (6%)	19	51
10	RO	100/100 (100%)	99 (99%)	1 (1%)	76	91
10	YO	100/100 (100%)	100 (100%)	0	100	100
11	RP	115/116 (99%)	110 (96%)	5 (4%)	29	63
11	YP	115/116 (99%)	109 (95%)	6 (5%)	23	57
12	RQ	111/111 (100%)	108 (97%)	3 (3%)	44	75
12	YQ	111/111 (100%)	107 (96%)	4 (4%)	35	68
13	RR	101/101 (100%)	95 (94%)	6 (6%)	19	51
13	YR	101/101 (100%)	95 (94%)	6 (6%)	19	51
14	RS	87/88 (99%)	84 (97%)	3 (3%)	37	70
14	YS	85/88 (97%)	82 (96%)	3 (4%)	36	69
15	RT	115/127 (91%)	110 (96%)	5 (4%)	29	63
15	YT	113/127 (89%)	109 (96%)	4 (4%)	36	69
16	RU	93/94 (99%)	91 (98%)	2 (2%)	52	79
16	YU	93/94 (99%)	92 (99%)	1 (1%)	73	90
17	RV	81/82 (99%)	77 (95%)	4 (5%)	25	59
17	YV	80/82 (98%)	76 (95%)	4 (5%)	24	58
18	RW	90/92 (98%)	86 (96%)	4 (4%)	28	63
18	YW	90/92 (98%)	86 (96%)	4 (4%)	28	63

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
19	RX	77/78 (99%)	76 (99%)	1 (1%)	69	88
19	YX	77/78 (99%)	76 (99%)	1 (1%)	69	88
20	RY	86/91 (94%)	85 (99%)	1 (1%)	71	89
20	YY	86/91 (94%)	84 (98%)	2 (2%)	50	78
21	RZ	169/179 (94%)	165 (98%)	4 (2%)	49	78
21	YZ	165/179 (92%)	163 (99%)	2 (1%)	71	89
22	R0	61/67 (91%)	59 (97%)	2 (3%)	38	71
22	Y0	61/67 (91%)	61 (100%)	0	100	100
23	R1	79/83 (95%)	76 (96%)	3 (4%)	33	67
23	Y1	81/83 (98%)	77 (95%)	4 (5%)	25	59
24	R2	65/67 (97%)	65 (100%)	0	100	100
24	Y2	66/67 (98%)	66 (100%)	0	100	100
25	R3	51/52 (98%)	48 (94%)	3 (6%)	19	51
25	Y3	50/52 (96%)	47 (94%)	3 (6%)	19	51
26	R4	58/63 (92%)	56 (97%)	2 (3%)	37	70
26	Y4	54/63 (86%)	50 (93%)	4 (7%)	13	42
27	R5	51/52 (98%)	48 (94%)	3 (6%)	19	51
27	Y5	50/52 (96%)	47 (94%)	3 (6%)	19	51
28	R6	51/52 (98%)	49 (96%)	2 (4%)	32	66
28	Y6	50/52 (96%)	49 (98%)	1 (2%)	55	81
29	R7	41/42 (98%)	39 (95%)	2 (5%)	25	59
29	Y7	41/42 (98%)	39 (95%)	2 (5%)	25	59
30	R8	54/55 (98%)	51 (94%)	3 (6%)	21	54
30	Y8	54/55 (98%)	51 (94%)	3 (6%)	21	54
31	R9	34/34 (100%)	34 (100%)	0	100	100
31	Y9	34/34 (100%)	34 (100%)	0	100	100
33	QB	191/220 (87%)	177 (93%)	14 (7%)	14	42
33	XB	187/220 (85%)	173 (92%)	14 (8%)	13	41
34	QC	144/188 (77%)	138 (96%)	6 (4%)	30	64
34	XC	140/188 (74%)	133 (95%)	7 (5%)	24	58
35	QD	171/181 (94%)	166 (97%)	5 (3%)	42	74

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
35	XD	172/181 (95%)	163 (95%)	9 (5%)	23	57
36	QE	114/123 (93%)	112 (98%)	2 (2%)	59	83
36	XE	114/123 (93%)	110 (96%)	4 (4%)	36	69
37	QF	85/90 (94%)	85 (100%)	0	100	100
37	XF	85/90 (94%)	84 (99%)	1 (1%)	71	89
38	QG	120/127 (94%)	115 (96%)	5 (4%)	30	64
38	XG	119/127 (94%)	116 (98%)	3 (2%)	47	77
39	QH	116/119 (98%)	112 (97%)	4 (3%)	37	70
39	XH	114/119 (96%)	111 (97%)	3 (3%)	46	76
40	QI	91/99 (92%)	85 (93%)	6 (7%)	16	47
40	XI	88/99 (89%)	83 (94%)	5 (6%)	20	53
41	QJ	68/92 (74%)	67 (98%)	1 (2%)	65	86
41	XJ	68/92 (74%)	68 (100%)	0	100	100
42	QK	83/99 (84%)	80 (96%)	3 (4%)	35	68
42	XK	83/99 (84%)	80 (96%)	3 (4%)	35	68
43	QL	96/108 (89%)	96 (100%)	0	100	100
43	XL	96/108 (89%)	92 (96%)	4 (4%)	30	64
44	QM	90/101 (89%)	88 (98%)	2 (2%)	52	79
44	XM	87/101 (86%)	84 (97%)	3 (3%)	37	70
45	QN	49/50 (98%)	45 (92%)	4 (8%)	11	37
45	XN	49/50 (98%)	48 (98%)	1 (2%)	55	81
46	QO	78/80 (98%)	77 (99%)	1 (1%)	69	88
46	XO	78/80 (98%)	76 (97%)	2 (3%)	46	76
47	QP	69/74 (93%)	66 (96%)	3 (4%)	29	63
47	XP	68/74 (92%)	64 (94%)	4 (6%)	19	51
48	QQ	94/97 (97%)	93 (99%)	1 (1%)	73	90
48	XQ	94/97 (97%)	92 (98%)	2 (2%)	53	80
49	QR	59/77 (77%)	57 (97%)	2 (3%)	37	70
49	XR	59/77 (77%)	58 (98%)	1 (2%)	60	84
50	QS	68/80 (85%)	65 (96%)	3 (4%)	28	63
50	XS	67/80 (84%)	67 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
51	QT	71/82 (87%)	67 (94%)	4 (6%)	21	54
51	XT	70/82 (85%)	67 (96%)	3 (4%)	29	63
52	QU	18/22 (82%)	18 (100%)	0	100	100
52	XU	18/22 (82%)	17 (94%)	1 (6%)	21	54
55	QY	210/300 (70%)	206 (98%)	4 (2%)	57	82
55	XY	211/300 (70%)	202 (96%)	9 (4%)	29	63
All	All	9784/10664 (92%)	9432 (96%)	352 (4%)	35	68

All (352) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	RD	52	ARG
3	RD	142	VAL
3	RD	211	ARG
3	RD	257	LEU
4	RE	9	VAL
4	RE	21	VAL
4	RE	75	VAL
4	RE	111	ARG
4	RE	113	PHE
4	RE	116	VAL
4	RE	184	VAL
5	RF	20	LEU
5	RF	33	LEU
5	RF	53	THR
5	RF	57	VAL
5	RF	110	LEU
5	RF	125	LEU
5	RF	168	ARG
5	RF	192	LEU
5	RF	197	ASP
6	RG	7	LEU
6	RG	60	LEU
6	RG	82	LEU
6	RG	146	TYR
6	RG	170	ARG
7	RH	23	ARG
7	RH	62	LYS
7	RH	105	LEU
8	RI	12	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
8	RI	57	ARG
8	RI	75	LEU
8	RI	109	ILE
8	RI	121	LYS
9	RN	12	ARG
9	RN	48	MET
9	RN	61	ARG
9	RN	99	LEU
9	RN	120	LEU
9	RN	121	LYS
10	RO	69	ILE
11	RP	55	ARG
11	RP	59	LEU
11	RP	65	ARG
11	RP	106	LEU
11	RP	112	LEU
12	RQ	16	ARG
12	RQ	75	THR
12	RQ	109	VAL
13	RR	18	LEU
13	RR	28	LEU
13	RR	44	LEU
13	RR	60	LEU
13	RR	79	LEU
13	RR	86	ARG
14	RS	23	ARG
14	RS	25	ARG
14	RS	59	LYS
15	RT	16	ARG
15	RT	53	ARG
15	RT	64	ARG
15	RT	78	LEU
15	RT	96	ARG
16	RU	74	LEU
16	RU	92	ARG
17	RV	18	LEU
17	RV	61	VAL
17	RV	79	VAL
17	RV	82	ARG
18	RW	4	LYS
18	RW	11	ARG
18	RW	51	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
18	RW	67	ASP
19	RX	76	ARG
20	RY	90	LEU
21	RZ	28	MET
21	RZ	150	LEU
21	RZ	161	VAL
21	RZ	185	GLU
22	R0	39	ARG
22	R0	59	LEU
23	R1	21	ARG
23	R1	52	ARG
23	R1	95	LEU
25	R3	8	LEU
25	R3	44	ARG
25	R3	54	VAL
26	R4	49	PHE
26	R4	61	ARG
27	R5	29	THR
27	R5	35	GLU
27	R5	60	VAL
28	R6	19	ARG
28	R6	28	ARG
29	R7	23	ARG
29	R7	43	THR
30	R8	30	ARG
30	R8	31	HIS
30	R8	34	TRP
33	QB	15	VAL
33	QB	16	HIS
33	QB	21	ARG
33	QB	24	TRP
33	QB	44	LEU
33	QB	76	GLN
33	QB	106	LYS
33	QB	122	PHE
33	QB	135	GLN
33	QB	144	ARG
33	QB	157	ARG
33	QB	160	ASP
33	QB	163	PHE
33	QB	195	ASP
34	QC	29	TYR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
34	QC	36	ASP
34	QC	127	ARG
34	QC	150	LYS
34	QC	178	LEU
34	QC	196	LEU
35	QD	8	VAL
35	QD	31	CYS
35	QD	49	ARG
35	QD	115	ARG
35	QD	135	LEU
36	QE	12	LEU
36	QE	41	VAL
38	QG	56	GLN
38	QG	73	MET
38	QG	104	LEU
38	QG	114	ARG
38	QG	143	ARG
39	QH	18	ARG
39	QH	25	ASP
39	QH	56	LYS
39	QH	112	LEU
40	QI	42	ARG
40	QI	66	ARG
40	QI	81	ILE
40	QI	83	ARG
40	QI	92	TYR
40	QI	93	ARG
41	QJ	84	GLN
42	QK	96	ARG
42	QK	116	HIS
42	QK	117	ASN
44	QM	3	ARG
44	QM	65	LYS
45	QN	3	ARG
45	QN	18	VAL
45	QN	33	VAL
45	QN	41	ARG
46	QO	39	LEU
47	QP	19	ILE
47	QP	20	VAL
47	QP	50	LYS
48	QQ	72	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
49	QR	31	LEU
49	QR	76	LEU
50	QS	5	LEU
50	QS	41	VAL
50	QS	65	ASN
51	QT	9	ASN
51	QT	10	LEU
51	QT	84	LEU
51	QT	100	ILE
55	QY	184	VAL
55	QY	244	ILE
55	QY	305	ASP
55	QY	311	ASN
3	YD	69	ARG
3	YD	94	LEU
3	YD	142	VAL
3	YD	211	ARG
3	YD	257	LEU
3	YD	275	LYS
4	YE	9	VAL
4	YE	21	VAL
4	YE	52	LEU
4	YE	75	VAL
4	YE	111	ARG
4	YE	113	PHE
4	YE	116	VAL
5	YF	20	LEU
5	YF	33	LEU
5	YF	57	VAL
5	YF	110	LEU
5	YF	183	VAL
5	YF	197	ASP
6	YG	3	LEU
6	YG	21	ARG
6	YG	49	ASP
6	YG	113	ARG
6	YG	115	ARG
6	YG	136	ARG
6	YG	146	TYR
6	YG	170	ARG
7	YH	23	ARG
7	YH	30	LYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
7	YH	33	LEU
7	YH	71	LEU
7	YH	88	LEU
8	YI	9	LEU
8	YI	50	ARG
8	YI	61	ARG
8	YI	68	LEU
8	YI	75	LEU
8	YI	77	LEU
8	YI	92	VAL
8	YI	116	LEU
8	YI	123	LEU
9	YN	12	ARG
9	YN	28	THR
9	YN	67	LEU
9	YN	87	LEU
9	YN	96	GLU
9	YN	99	LEU
9	YN	120	LEU
11	YP	55	ARG
11	YP	59	LEU
11	YP	65	ARG
11	YP	106	LEU
11	YP	112	LEU
11	YP	148	LEU
12	YQ	16	ARG
12	YQ	21	THR
12	YQ	75	THR
12	YQ	109	VAL
13	YR	18	LEU
13	YR	28	LEU
13	YR	44	LEU
13	YR	60	LEU
13	YR	79	LEU
13	YR	111	LEU
14	YS	23	ARG
14	YS	25	ARG
14	YS	67	ARG
15	YT	16	ARG
15	YT	64	ARG
15	YT	95	ARG
15	YT	96	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
16	YU	74	LEU
17	YV	38	LEU
17	YV	53	GLU
17	YV	79	VAL
17	YV	82	ARG
18	YW	11	ARG
18	YW	15	ARG
18	YW	23	LEU
18	YW	51	LEU
19	YX	88	LYS
20	YY	23	ARG
20	YY	72	VAL
21	YZ	94	GLU
21	YZ	150	LEU
23	Y1	21	ARG
23	Y1	26	ARG
23	Y1	52	ARG
23	Y1	96	LYS
25	Y3	8	LEU
25	Y3	30	ARG
25	Y3	54	VAL
26	Y4	8	LYS
26	Y4	48	ARG
26	Y4	58	ARG
26	Y4	62	ARG
27	Y5	29	THR
27	Y5	35	GLU
27	Y5	40	LYS
28	Y6	19	ARG
29	Y7	23	ARG
29	Y7	43	THR
30	Y8	30	ARG
30	Y8	31	HIS
30	Y8	34	TRP
33	XB	16	HIS
33	XB	17	PHE
33	XB	24	TRP
33	XB	44	LEU
33	XB	114	ARG
33	XB	122	PHE
33	XB	127	ILE
33	XB	154	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
33	XB	157	ARG
33	XB	160	ASP
33	XB	163	PHE
33	XB	217	ARG
33	XB	224	GLN
33	XB	226	ARG
34	XC	29	TYR
34	XC	30	ARG
34	XC	45	LYS
34	XC	85	ARG
34	XC	140	ARG
34	XC	178	LEU
34	XC	190	ARG
35	XD	8	VAL
35	XD	28	SER
35	XD	31	CYS
35	XD	65	ARG
35	XD	108	LEU
35	XD	115	ARG
35	XD	118	ARG
35	XD	135	LEU
35	XD	150	GLU
36	XE	41	VAL
36	XE	68	GLU
36	XE	72	GLN
36	XE	143	ARG
37	XF	72	VAL
38	XG	90	GLU
38	XG	104	LEU
38	XG	115	ARG
39	XH	14	ARG
39	XH	69	ARG
39	XH	112	LEU
40	XI	23	ASN
40	XI	35	GLU
40	XI	83	ARG
40	XI	92	TYR
40	XI	102	LEU
42	XK	96	ARG
42	XK	116	HIS
42	XK	117	ASN
43	XL	41	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
43	XL	52	LEU
43	XL	86	ARG
43	XL	117	ARG
44	XM	63	THR
44	XM	69	GLU
44	XM	110	ARG
45	XN	18	VAL
46	XO	54	ARG
46	XO	83	GLU
47	XP	20	VAL
47	XP	28	ARG
47	XP	54	GLU
47	XP	60	LEU
48	XQ	72	ARG
48	XQ	74	LEU
49	XR	41	LYS
51	XT	84	LEU
51	XT	89	ARG
51	XT	100	ILE
52	XU	15	ARG
55	XY	99	LEU
55	XY	100	LEU
55	XY	101	LEU
55	XY	103	LYS
55	XY	104	ASP
55	XY	249	LEU
55	XY	259	ASP
55	XY	318	THR
55	XY	340	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
18	RW	60	ASN
20	RY	6	HIS
33	QB	78	GLN
33	QB	95	GLN
50	QS	65	ASN
6	YG	79	ASN
15	YT	58	ASN
20	YY	6	HIS
33	XB	78	GLN

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Mol	Chain	Res	Type
47	XP	14	ASN
47	XP	16	HIS

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	RA	2855/2915 (97%)	494 (17%)	22 (0%)
1	YA	2855/2915 (97%)	484 (16%)	24 (0%)
2	RB	119/122 (97%)	14 (11%)	0
2	YB	119/122 (97%)	13 (10%)	0
32	QA	1494/1521 (98%)	257 (17%)	15 (1%)
32	XA	1498/1521 (98%)	234 (15%)	16 (1%)
53	QV	76/77 (98%)	16 (21%)	0
53	XV	76/77 (98%)	16 (21%)	1 (1%)
54	QX	8/25 (32%)	4 (50%)	0
54	XX	9/25 (36%)	4 (44%)	0
All	All	9109/9320 (97%)	1536 (16%)	78 (0%)

All (1536) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	RA	10	G
1	RA	12	U
1	RA	36	G
1	RA	45	C
1	RA	59	U
1	RA	61	G
1	RA	71	A
1	RA	74	A
1	RA	75	G
1	RA	83	G
1	RA	84	A
1	RA	92	A
1	RA	95	G
1	RA	102	G
1	RA	118	A
1	RA	119	A
1	RA	120	U
1	RA	125	G
1	RA	128	C
1	RA	141	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	RA	157	U
1	RA	181	A
1	RA	182	A
1	RA	196	A
1	RA	199	A
1	RA	201	C
1	RA	205	G
1	RA	214	G
1	RA	215	G
1	RA	216	A
1	RA	221	A
1	RA	222	A
1	RA	225	A
1	RA	229	A
1	RA	230	U
1	RA	232	G
1	RA	248	G
1	RA	250	G
1	RA	272(K)	U
1	RA	272(L)	U
1	RA	272(M)	G
1	RA	272(N)	U
1	RA	272(O)	C
1	RA	273(B)	U
1	RA	273(C)	G
1	RA	273(K)	C
1	RA	277	C
1	RA	278	A
1	RA	311	A
1	RA	317	G
1	RA	324	A
1	RA	327	G
1	RA	329	G
1	RA	330	A
1	RA	352	G
1	RA	363(A)	G
1	RA	372	G
1	RA	386	G
1	RA	396	G
1	RA	405	U
1	RA	407	G
1	RA	411	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	RA	428	A
1	RA	444	C
1	RA	456	C
1	RA	457	A
1	RA	470	A
1	RA	481	G
1	RA	482	A
1	RA	494	G
1	RA	496	G
1	RA	504	U
1	RA	505	A
1	RA	508	G
1	RA	509	C
1	RA	530	G
1	RA	531	C
1	RA	532	A
1	RA	533	G
1	RA	545	G
1	RA	556	G
1	RA	563	G
1	RA	567	A
1	RA	568	U
1	RA	573	G
1	RA	575	A
1	RA	586	A
1	RA	587	C
1	RA	595	C
1	RA	603	A
1	RA	604	G
1	RA	607	U
1	RA	614(C)	G
1	RA	615	G
1	RA	627	A
1	RA	637	A
1	RA	645	C
1	RA	646	A
1	RA	652(C)	A
1	RA	652(D)	G
1	RA	652(V)	G
1	RA	653	A
1	RA	669	G
1	RA	686	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	RA	715	G
1	RA	729	G
1	RA	730	C
1	RA	753	C
1	RA	764	A
1	RA	775	G
1	RA	776	G
1	RA	782	A
1	RA	784	A
1	RA	785	G
1	RA	792	G
1	RA	805	G
1	RA	812	C
1	RA	827	U
1	RA	828	U
1	RA	857	C
1	RA	859	G
1	RA	869	G
1	RA	877	U
1	RA	880	G
1	RA	886	C
1	RA	887	A
1	RA	888	C
1	RA	889	C
1	RA	890	A
1	RA	893	C
1	RA	896	A
1	RA	897	C
1	RA	900	A
1	RA	907	U
1	RA	910	A
1	RA	914	C
1	RA	915	C
1	RA	917	A
1	RA	926	A
1	RA	932	G
1	RA	936	C
1	RA	941	A
1	RA	945	A
1	RA	946	G
1	RA	953	A
1	RA	959	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	RA	961	C
1	RA	974	G
1	RA	975(A)	C
1	RA	983	A
1	RA	996	A
1	RA	1008	C
1	RA	1012	U
1	RA	1013	C
1	RA	1017	G
1	RA	1025	G
1	RA	1026	U
1	RA	1033	U
1	RA	1034	G
1	RA	1038	C
1	RA	1039	G
1	RA	1043	C
1	RA	1044	G
1	RA	1045	A
1	RA	1046	A
1	RA	1047	G
1	RA	1048	A
1	RA	1049	C
1	RA	1053	C
1	RA	1054	A
1	RA	1055	G
1	RA	1058	G
1	RA	1060	U
1	RA	1063	G
1	RA	1064	C
1	RA	1065	U
1	RA	1066	U
1	RA	1067	A
1	RA	1068	G
1	RA	1069	A
1	RA	1070	A
1	RA	1071	G
1	RA	1073	A
1	RA	1074	G
1	RA	1076	C
1	RA	1078	U
1	RA	1079	C
1	RA	1082	U

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	RA	1083	U
1	RA	1084	A
1	RA	1085	A
1	RA	1086	A
1	RA	1087	G
1	RA	1088	A
1	RA	1090	U
1	RA	1091	G
1	RA	1092	C
1	RA	1094	U
1	RA	1096	A
1	RA	1097	U
1	RA	1098	A
1	RA	1100	C
1	RA	1109	C
1	RA	1110	G
1	RA	1111	A
1	RA	1112	G
1	RA	1129	A
1	RA	1130	U
1	RA	1135	C
1	RA	1136	G
1	RA	1138	G
1	RA	1142(B)	A
1	RA	1170	G
1	RA	1171	G
1	RA	1211	U
1	RA	1219	G
1	RA	1236	G
1	RA	1241	A
1	RA	1248	G
1	RA	1250	G
1	RA	1253	A
1	RA	1256	G
1	RA	1271	G
1	RA	1272	A
1	RA	1300	U
1	RA	1301	A
1	RA	1306	C
1	RA	1309	G
1	RA	1314	C
1	RA	1320	C

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	RA	1321	A
1	RA	1352	U
1	RA	1359	A
1	RA	1360	A
1	RA	1365	A
1	RA	1368	G
1	RA	1378	A
1	RA	1384	A
1	RA	1385	G
1	RA	1395	A
1	RA	1416	G
1	RA	1417	C
1	RA	1420	U
1	RA	1421	G
1	RA	1427	A
1	RA	1428	C
1	RA	1445(A)	A
1	RA	1450(A)	G
1	RA	1455	G
1	RA	1459	G
1	RA	1460	A
1	RA	1467	C
1	RA	1471	A
1	RA	1482	G
1	RA	1493	C
1	RA	1497	U
1	RA	1508	A
1	RA	1509(A)	C
1	RA	1509(B)	A
1	RA	1509(C)	A
1	RA	1531	C
1	RA	1542	A
1	RA	1543	C
1	RA	1554	A
1	RA	1558	A
1	RA	1566	A
1	RA	1569	A
1	RA	1578	U
1	RA	1580	A
1	RA	1584	C
1	RA	1586	A
1	RA	1608	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	RA	1609	A
1	RA	1618	A
1	RA	1640	C
1	RA	1648	C
1	RA	1654	A
1	RA	1674	G
1	RA	1675	C
1	RA	1696	G
1	RA	1698	A
1	RA	1700	A
1	RA	1701	A
1	RA	1703	G
1	RA	1721	G
1	RA	1722	A
1	RA	1746	G
1	RA	1756	G
1	RA	1762	A
1	RA	1763	G
1	RA	1764	G
1	RA	1773	A
1	RA	1776	G
1	RA	1780	A
1	RA	1782	C
1	RA	1784	A
1	RA	1791	A
1	RA	1800	C
1	RA	1801	G
1	RA	1812	A
1	RA	1816	G
1	RA	1833	U
1	RA	1835	G
1	RA	1847	A
1	RA	1848	A
1	RA	1877	A
1	RA	1878	G
1	RA	1889	A
1	RA	1895	C
1	RA	1900	A
1	RA	1906	G
1	RA	1913	A
1	RA	1914	C
1	RA	1929	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	RA	1930	G
1	RA	1936	A
1	RA	1937	A
1	RA	1938	A
1	RA	1939	5MU
1	RA	1955	U
1	RA	1960	A
1	RA	1963	U
1	RA	1967	C
1	RA	1970	A
1	RA	1971	A
1	RA	1972	A
1	RA	1975	G
1	RA	1993	U
1	RA	1997	G
1	RA	2023	G
1	RA	2031	A
1	RA	2032	G
1	RA	2033	A
1	RA	2037	G
1	RA	2043	C
1	RA	2055	C
1	RA	2056	G
1	RA	2060	A
1	RA	2061	G
1	RA	2062	A
1	RA	2063	C
1	RA	2069	G
1	RA	2096	U
1	RA	2099	U
1	RA	2103	C
1	RA	2104	G
1	RA	2105	C
1	RA	2107	C
1	RA	2108	C
1	RA	2109	U
1	RA	2112	G
1	RA	2114	A
1	RA	2116	G
1	RA	2117	A
1	RA	2119	A
1	RA	2121	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	RA	2123	G
1	RA	2126	A
1	RA	2127	G
1	RA	2129	C
1	RA	2131	G
1	RA	2132	U
1	RA	2133	G
1	RA	2134	A
1	RA	2135	A
1	RA	2136	C
1	RA	2138	C
1	RA	2145	C
1	RA	2146	C
1	RA	2147	G
1	RA	2148	G
1	RA	2151	G
1	RA	2157	G
1	RA	2158	A
1	RA	2159	G
1	RA	2161	C
1	RA	2165	G
1	RA	2172	U
1	RA	2173	A
1	RA	2174	C
1	RA	2180	U
1	RA	2186	G
1	RA	2189	U
1	RA	2192	G
1	RA	2198	A
1	RA	2206	G
1	RA	2207	G
1	RA	2208	A
1	RA	2218	U
1	RA	2219	G
1	RA	2225	A
1	RA	2238	G
1	RA	2239	G
1	RA	2243	U
1	RA	2269	A
1	RA	2275	C
1	RA	2278	A
1	RA	2283	C

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	RA	2287	A
1	RA	2291	U
1	RA	2292	C
1	RA	2305	A
1	RA	2308	G
1	RA	2309	A
1	RA	2311	A
1	RA	2312	U
1	RA	2319	G
1	RA	2320	A
1	RA	2321	G
1	RA	2322	A
1	RA	2325	G
1	RA	2334	G
1	RA	2335	A
1	RA	2336	A
1	RA	2343	C
1	RA	2347	C
1	RA	2350	C
1	RA	2372	G
1	RA	2379	G
1	RA	2383	G
1	RA	2385	C
1	RA	2400	G
1	RA	2406	U
1	RA	2410	G
1	RA	2414	G
1	RA	2422	A
1	RA	2424	C
1	RA	2425	A
1	RA	2429	G
1	RA	2430	A
1	RA	2434	A
1	RA	2435	A
1	RA	2439	A
1	RA	2441	C
1	RA	2448	A
1	RA	2474	C
1	RA	2475	C
1	RA	2476	A
1	RA	2478	A
1	RA	2498	C

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	RA	2502	G
1	RA	2504	U
1	RA	2505	G
1	RA	2518	A
1	RA	2520	C
1	RA	2529	G
1	RA	2549	G
1	RA	2554	U
1	RA	2555	U
1	RA	2566	A
1	RA	2567	G
1	RA	2601	C
1	RA	2602	A
1	RA	2609	U
1	RA	2611	U
1	RA	2612	C
1	RA	2615	U
1	RA	2629	A
1	RA	2630	G
1	RA	2632	A
1	RA	2654	A
1	RA	2689	U
1	RA	2690	C
1	RA	2691	C
1	RA	2700	C
1	RA	2702	U
1	RA	2703	C
1	RA	2712(B)	A
1	RA	2713	A
1	RA	2714	G
1	RA	2726	U
1	RA	2733	A
1	RA	2744	G
1	RA	2751	G
1	RA	2758	A
1	RA	2759	G
1	RA	2764	A
1	RA	2765	A
1	RA	2766	G
1	RA	2778	A
1	RA	2789	C
1	RA	2794(A)	C

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	RA	2818	G
1	RA	2820	A
1	RA	2821	A
1	RA	2833	G
1	RA	2872	G
1	RA	2873	A
1	RA	2879	C
1	RA	2880	C
1	RA	2886	G
1	RA	2892	A
1	RA	2894	G
1	RA	2897	U
2	RB	2	C
2	RB	7	G
2	RB	8	U
2	RB	13	A
2	RB	24	G
2	RB	30	C
2	RB	34	U
2	RB	45	A
2	RB	53	A
2	RB	56	G
2	RB	73	A
2	RB	85	G
2	RB	106	G
2	RB	110	G
32	QA	5	U
32	QA	7	G
32	QA	9	G
32	QA	32	A
32	QA	39	G
32	QA	41	G
32	QA	42	G
32	QA	48	C
32	QA	50	A
32	QA	51	A
32	QA	53	A
32	QA	61	G
32	QA	78	G
32	QA	79	G
32	QA	101	A
32	QA	116	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
32	QA	121	C
32	QA	127	G
32	QA	131	C
32	QA	137	C
32	QA	163	C
32	QA	169	C
32	QA	174	C
32	QA	182	U
32	QA	189(F)	U
32	QA	195	A
32	QA	201	C
32	QA	203	U
32	QA	204	U
32	QA	216	G
32	QA	231	G
32	QA	247	G
32	QA	251	G
32	QA	266	G
32	QA	267	C
32	QA	289	G
32	QA	298	A
32	QA	306	G
32	QA	321	A
32	QA	328	C
32	QA	332	G
32	QA	343	U
32	QA	345	C
32	QA	347	G
32	QA	348	G
32	QA	352	C
32	QA	353	A
32	QA	354	G
32	QA	367	U
32	QA	372	C
32	QA	373	A
32	QA	384	G
32	QA	397	A
32	QA	406	G
32	QA	412	A
32	QA	413	G
32	QA	423	G
32	QA	424	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
32	QA	429	U
32	QA	439	A
32	QA	442	C
32	QA	446	G
32	QA	452	A
32	QA	454	C
32	QA	458	C
32	QA	461	A
32	QA	470	C
32	QA	477	A
32	QA	485	G
32	QA	496	A
32	QA	498	U
32	QA	505	G
32	QA	509	A
32	QA	510	A
32	QA	511	C
32	QA	513	C
32	QA	517	G
32	QA	518	C
32	QA	521	G
32	QA	524	G
32	QA	527	7MG
32	QA	532	A
32	QA	547	A
32	QA	550	G
32	QA	559	A
32	QA	561	U
32	QA	564	C
32	QA	572	A
32	QA	573	A
32	QA	574	A
32	QA	575	G
32	QA	576	G
32	QA	577	G
32	QA	596	C
32	QA	607	A
32	QA	619	U
32	QA	630	G
32	QA	631	G
32	QA	632	A
32	QA	653	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
32	QA	661	G
32	QA	665	A
32	QA	687	A
32	QA	688	G
32	QA	721	G
32	QA	723	U
32	QA	731	G
32	QA	755	G
32	QA	760	G
32	QA	774	G
32	QA	777	A
32	QA	787	A
32	QA	792	A
32	QA	793	U
32	QA	794	A
32	QA	796	C
32	QA	798	G
32	QA	816	A
32	QA	817	C
32	QA	821	G
32	QA	828	A
32	QA	829	G
32	QA	839	U
32	QA	840	C
32	QA	841	U
32	QA	848	C
32	QA	851	G
32	QA	902	G
32	QA	914	A
32	QA	916	G
32	QA	917	G
32	QA	926	G
32	QA	927	G
32	QA	934	C
32	QA	935	A
32	QA	939	G
32	QA	942	G
32	QA	944	G
32	QA	960	U
32	QA	961	U
32	QA	968	A
32	QA	969	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
32	QA	971	G
32	QA	974	A
32	QA	975	A
32	QA	976	G
32	QA	977	A
32	QA	992	U
32	QA	993	G
32	QA	994	A
32	QA	998	G
32	QA	1003	G
32	QA	1006	C
32	QA	1009	G
32	QA	1022	G
32	QA	1023	G
32	QA	1024	G
32	QA	1025	U
32	QA	1026	G
32	QA	1027	C
32	QA	1028	C
32	QA	1029	C
32	QA	1030(A)	C
32	QA	1030(B)	G
32	QA	1030(C)	C
32	QA	1030(E)	A
32	QA	1032	G
32	QA	1034	G
32	QA	1037	C
32	QA	1044	A
32	QA	1053	G
32	QA	1065	U
32	QA	1066	C
32	QA	1068	G
32	QA	1070	U
32	QA	1081	G
32	QA	1087	G
32	QA	1094	G
32	QA	1095	U
32	QA	1101	A
32	QA	1108	G
32	QA	1113	C
32	QA	1125	U
32	QA	1126	U

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
32	QA	1130	A
32	QA	1134	G
32	QA	1136	U
32	QA	1138	G
32	QA	1139	G
32	QA	1146	A
32	QA	1152	A
32	QA	1159	U
32	QA	1168	A
32	QA	1183	A
32	QA	1184	G
32	QA	1193	G
32	QA	1196	U
32	QA	1197	G
32	QA	1202	G
32	QA	1204	A
32	QA	1208	C
32	QA	1212	U
32	QA	1213	A
32	QA	1225	A
32	QA	1227	A
32	QA	1238	A
32	QA	1256	A
32	QA	1257	U
32	QA	1258	G
32	QA	1278	U
32	QA	1280	A
32	QA	1286	A
32	QA	1287	A
32	QA	1299	A
32	QA	1300	G
32	QA	1302	U
32	QA	1305	G
32	QA	1311	G
32	QA	1319	A
32	QA	1320	C
32	QA	1338	G
32	QA	1340	A
32	QA	1347	G
32	QA	1353	G
32	QA	1359	C
32	QA	1363(A)	C

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
32	QA	1363(B)	A
32	QA	1364	U
32	QA	1370	G
32	QA	1379	G
32	QA	1381	U
32	QA	1397	C
32	QA	1398	A
32	QA	1401	G
32	QA	1419	G
32	QA	1442(A)	G
32	QA	1442(B)	G
32	QA	1442(C)	A
32	QA	1446	U
32	QA	1447	A
32	QA	1452	C
32	QA	1456	G
32	QA	1487	G
32	QA	1491	G
32	QA	1492	A
32	QA	1493	A
32	QA	1497	G
32	QA	1499	A
32	QA	1503	A
32	QA	1504	G
32	QA	1505	G
32	QA	1506	U
32	QA	1507	A
32	QA	1517	G
32	QA	1520	G
32	QA	1529	G
32	QA	1530	G
53	QV	4	G
53	QV	5	G
53	QV	8	U
53	QV	9	G
53	QV	17(A)	U
53	QV	18	G
53	QV	19	G
53	QV	21	A
53	QV	22	G
53	QV	31	G
53	QV	47	U

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
53	QV	48	C
53	QV	54	U
53	QV	68	C
53	QV	75	C
53	QV	76	A
54	QX	15	A
54	QX	17	U
54	QX	21	A
54	QX	22	C
1	YA	9	U
1	YA	10	G
1	YA	12	U
1	YA	15	G
1	YA	34	C
1	YA	45	C
1	YA	55	G
1	YA	71	A
1	YA	74	A
1	YA	75	G
1	YA	84	A
1	YA	92	A
1	YA	95	G
1	YA	118	A
1	YA	119	A
1	YA	120	U
1	YA	154(A)	G
1	YA	154(B)	C
1	YA	157	U
1	YA	181	A
1	YA	182	A
1	YA	188	G
1	YA	196	A
1	YA	199	A
1	YA	205	G
1	YA	214	G
1	YA	215	G
1	YA	216	A
1	YA	221	A
1	YA	222	A
1	YA	229	A
1	YA	230	U
1	YA	233	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	YA	248	G
1	YA	266	G
1	YA	272(K)	U
1	YA	272(L)	U
1	YA	272(M)	G
1	YA	272(N)	U
1	YA	272(O)	C
1	YA	273(B)	U
1	YA	273(C)	G
1	YA	273(K)	C
1	YA	277	C
1	YA	278	A
1	YA	311	A
1	YA	317	G
1	YA	324	A
1	YA	327	G
1	YA	329	G
1	YA	330	A
1	YA	342	G
1	YA	346	A
1	YA	352	G
1	YA	362	U
1	YA	363(A)	G
1	YA	372	G
1	YA	386	G
1	YA	389	G
1	YA	407	G
1	YA	411	G
1	YA	428	A
1	YA	444	C
1	YA	455	C
1	YA	463	G
1	YA	464	U
1	YA	470	A
1	YA	481	G
1	YA	505	A
1	YA	508	G
1	YA	509	C
1	YA	530	G
1	YA	531	C
1	YA	532	A
1	YA	533	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	YA	545	G
1	YA	563	G
1	YA	567	A
1	YA	573	G
1	YA	575	A
1	YA	586	A
1	YA	595	C
1	YA	603	A
1	YA	604	G
1	YA	607	U
1	YA	615	G
1	YA	616	G
1	YA	620	G
1	YA	627	A
1	YA	637	A
1	YA	644	A
1	YA	645	C
1	YA	646	A
1	YA	652(C)	A
1	YA	652(D)	G
1	YA	652(V)	G
1	YA	653	A
1	YA	669	G
1	YA	686	G
1	YA	715	G
1	YA	730	C
1	YA	747	U
1	YA	752	A
1	YA	753	C
1	YA	762	U
1	YA	775	G
1	YA	776	G
1	YA	782	A
1	YA	784	A
1	YA	785	G
1	YA	792	G
1	YA	805	G
1	YA	811	U
1	YA	812	C
1	YA	827	U
1	YA	828	U
1	YA	833	U

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	YA	859	G
1	YA	866	A
1	YA	878	A
1	YA	880	G
1	YA	886	C
1	YA	887	A
1	YA	888	C
1	YA	889	C
1	YA	890	A
1	YA	893	C
1	YA	896	A
1	YA	897	C
1	YA	899	A
1	YA	907	U
1	YA	910	A
1	YA	914	C
1	YA	917	A
1	YA	932	G
1	YA	941	A
1	YA	945	A
1	YA	946	G
1	YA	958	U
1	YA	959	A
1	YA	961	C
1	YA	962	G
1	YA	974	G
1	YA	975(A)	C
1	YA	983	A
1	YA	989	G
1	YA	996	A
1	YA	999	U
1	YA	1008	C
1	YA	1012	U
1	YA	1013	C
1	YA	1015	G
1	YA	1017	G
1	YA	1025	G
1	YA	1026	U
1	YA	1033	U
1	YA	1041	C
1	YA	1044	G
1	YA	1045	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	YA	1046	A
1	YA	1047	G
1	YA	1048	A
1	YA	1049	C
1	YA	1050	A
1	YA	1052	C
1	YA	1053	C
1	YA	1054	A
1	YA	1058	G
1	YA	1060	U
1	YA	1064	C
1	YA	1065	U
1	YA	1066	U
1	YA	1067	A
1	YA	1068	G
1	YA	1069	A
1	YA	1070	A
1	YA	1071	G
1	YA	1073	A
1	YA	1074	G
1	YA	1076	C
1	YA	1077	A
1	YA	1078	U
1	YA	1079	C
1	YA	1082	U
1	YA	1083	U
1	YA	1084	A
1	YA	1085	A
1	YA	1086	A
1	YA	1088	A
1	YA	1090	U
1	YA	1091	G
1	YA	1092	C
1	YA	1094	U
1	YA	1096	A
1	YA	1097	U
1	YA	1098	A
1	YA	1100	C
1	YA	1108	U
1	YA	1109	C
1	YA	1110	G
1	YA	1112	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	YA	1113	U
1	YA	1114	G
1	YA	1117	G
1	YA	1118	C
1	YA	1119	C
1	YA	1126	A
1	YA	1129	A
1	YA	1130	U
1	YA	1135	C
1	YA	1136	G
1	YA	1142(B)	A
1	YA	1151	G
1	YA	1155	A
1	YA	1157	G
1	YA	1171	G
1	YA	1211	U
1	YA	1212	G
1	YA	1220	A
1	YA	1236	G
1	YA	1250	G
1	YA	1253	A
1	YA	1256	G
1	YA	1271	G
1	YA	1272	A
1	YA	1273	U
1	YA	1300	U
1	YA	1301	A
1	YA	1313	U
1	YA	1314	C
1	YA	1352	U
1	YA	1359	A
1	YA	1365	A
1	YA	1368	G
1	YA	1378	A
1	YA	1380	G
1	YA	1384	A
1	YA	1385	G
1	YA	1386	C
1	YA	1416	G
1	YA	1417	C
1	YA	1420	U
1	YA	1421	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	YA	1428	C
1	YA	1445(A)	A
1	YA	1450(A)	G
1	YA	1451	C
1	YA	1455	G
1	YA	1459	G
1	YA	1467	C
1	YA	1471	A
1	YA	1478	G
1	YA	1482	G
1	YA	1490	A
1	YA	1493	C
1	YA	1497	U
1	YA	1508	A
1	YA	1509(A)	C
1	YA	1509(B)	A
1	YA	1531	C
1	YA	1542	A
1	YA	1543	C
1	YA	1547	C
1	YA	1554	A
1	YA	1558	A
1	YA	1559	G
1	YA	1566	A
1	YA	1569	A
1	YA	1578	U
1	YA	1580	A
1	YA	1584	C
1	YA	1586	A
1	YA	1608	A
1	YA	1609	A
1	YA	1610	A
1	YA	1640	C
1	YA	1648	C
1	YA	1651	G
1	YA	1664	A
1	YA	1674	G
1	YA	1675	C
1	YA	1696	G
1	YA	1700	A
1	YA	1701	A
1	YA	1703	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	YA	1721	G
1	YA	1722	A
1	YA	1756	G
1	YA	1762	A
1	YA	1763	G
1	YA	1764	G
1	YA	1773	A
1	YA	1776	G
1	YA	1780	A
1	YA	1782	C
1	YA	1786	A
1	YA	1791	A
1	YA	1800	C
1	YA	1801	G
1	YA	1812	A
1	YA	1816	G
1	YA	1829	A
1	YA	1834	U
1	YA	1835	G
1	YA	1847	A
1	YA	1848	A
1	YA	1877	A
1	YA	1878	G
1	YA	1890	A
1	YA	1900	A
1	YA	1906	G
1	YA	1914	C
1	YA	1929	G
1	YA	1930	G
1	YA	1937	A
1	YA	1938	A
1	YA	1955	U
1	YA	1963	U
1	YA	1965	C
1	YA	1967	C
1	YA	1970	A
1	YA	1971	A
1	YA	1972	A
1	YA	1993	U
1	YA	1997	G
1	YA	2020	A
1	YA	2023	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	YA	2031	A
1	YA	2032	G
1	YA	2033	A
1	YA	2043	C
1	YA	2055	C
1	YA	2056	G
1	YA	2060	A
1	YA	2061	G
1	YA	2062	A
1	YA	2069	G
1	YA	2096	U
1	YA	2099	U
1	YA	2103	C
1	YA	2105	C
1	YA	2107	C
1	YA	2108	C
1	YA	2109	U
1	YA	2112	G
1	YA	2116	G
1	YA	2117	A
1	YA	2118	U
1	YA	2119	A
1	YA	2121	G
1	YA	2123	G
1	YA	2126	A
1	YA	2127	G
1	YA	2128	C
1	YA	2129	C
1	YA	2131	G
1	YA	2132	U
1	YA	2133	G
1	YA	2134	A
1	YA	2136	C
1	YA	2138	C
1	YA	2145	C
1	YA	2146	C
1	YA	2147	G
1	YA	2151	G
1	YA	2158	A
1	YA	2159	G
1	YA	2161	C
1	YA	2165	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	YA	2172	U
1	YA	2173	A
1	YA	2180	U
1	YA	2186	G
1	YA	2189	U
1	YA	2192	G
1	YA	2198	A
1	YA	2206	G
1	YA	2207	G
1	YA	2208	A
1	YA	2218	U
1	YA	2225	A
1	YA	2238	G
1	YA	2239	G
1	YA	2269	A
1	YA	2275	C
1	YA	2279	G
1	YA	2283	C
1	YA	2287	A
1	YA	2305	A
1	YA	2308	G
1	YA	2312	U
1	YA	2320	A
1	YA	2321	G
1	YA	2322	A
1	YA	2325	G
1	YA	2334	G
1	YA	2335	A
1	YA	2336	A
1	YA	2343	C
1	YA	2347	C
1	YA	2350	C
1	YA	2372	G
1	YA	2383	G
1	YA	2384	G
1	YA	2385	C
1	YA	2389	G
1	YA	2400	G
1	YA	2406	U
1	YA	2410	G
1	YA	2414	G
1	YA	2422	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	YA	2425	A
1	YA	2429	G
1	YA	2430	A
1	YA	2431	U
1	YA	2435	A
1	YA	2439	A
1	YA	2441	C
1	YA	2448	A
1	YA	2468	G
1	YA	2474	C
1	YA	2476	A
1	YA	2487	G
1	YA	2502	G
1	YA	2504	U
1	YA	2505	G
1	YA	2518	A
1	YA	2520	C
1	YA	2525	G
1	YA	2529	G
1	YA	2530	A
1	YA	2549	G
1	YA	2554	U
1	YA	2566	A
1	YA	2567	G
1	YA	2578	G
1	YA	2582	G
1	YA	2602	A
1	YA	2609	U
1	YA	2611	U
1	YA	2612	C
1	YA	2629	A
1	YA	2630	G
1	YA	2636	U
1	YA	2654	A
1	YA	2663	G
1	YA	2682	U
1	YA	2689	U
1	YA	2690	C
1	YA	2691	C
1	YA	2702	U
1	YA	2703	C
1	YA	2712(B)	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	YA	2713	A
1	YA	2714	G
1	YA	2726	U
1	YA	2733	A
1	YA	2744	G
1	YA	2751	G
1	YA	2758	A
1	YA	2759	G
1	YA	2764	A
1	YA	2765	A
1	YA	2769	C
1	YA	2778	A
1	YA	2780	G
1	YA	2802	G
1	YA	2811	G
1	YA	2818	G
1	YA	2820	A
1	YA	2821	A
1	YA	2833	G
1	YA	2835	A
1	YA	2849	U
1	YA	2866	U
1	YA	2872	G
1	YA	2873	A
1	YA	2879	C
1	YA	2880	C
1	YA	2886	G
1	YA	2891	G
1	YA	2892	A
1	YA	2894	G
1	YA	2897	U
2	YB	8	U
2	YB	9	G
2	YB	12	C
2	YB	25	A
2	YB	30	C
2	YB	51	G
2	YB	56	G
2	YB	63	G
2	YB	73	A
2	YB	84	C
2	YB	106	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	YB	109	C
2	YB	110	G
32	XA	5	U
32	XA	7	G
32	XA	9	G
32	XA	32	A
32	XA	39	G
32	XA	47	C
32	XA	48	C
32	XA	50	A
32	XA	51	A
32	XA	61	G
32	XA	65	U
32	XA	66	G
32	XA	69	G
32	XA	78	G
32	XA	88	A
32	XA	89	C
32	XA	101	A
32	XA	116	A
32	XA	121	C
32	XA	131	C
32	XA	151	A
32	XA	163	C
32	XA	174	C
32	XA	182	U
32	XA	189(F)	U
32	XA	195	A
32	XA	197	A
32	XA	202	U
32	XA	203	U
32	XA	204	U
32	XA	216	G
32	XA	247	G
32	XA	251	G
32	XA	262	A
32	XA	266	G
32	XA	267	C
32	XA	281	G
32	XA	289	G
32	XA	321	A
32	XA	328	C

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
32	XA	332	G
32	XA	340	U
32	XA	351	G
32	XA	352	C
32	XA	353	A
32	XA	354	G
32	XA	356	A
32	XA	367	U
32	XA	372	C
32	XA	373	A
32	XA	384	G
32	XA	397	A
32	XA	398	C
32	XA	406	G
32	XA	412	A
32	XA	413	G
32	XA	424	G
32	XA	429	U
32	XA	439	A
32	XA	442	C
32	XA	452	A
32	XA	458	C
32	XA	470	C
32	XA	482	A
32	XA	484	G
32	XA	485	G
32	XA	496	A
32	XA	498	U
32	XA	505	G
32	XA	509	A
32	XA	510	A
32	XA	511	C
32	XA	518	C
32	XA	527	7MG
32	XA	532	A
32	XA	533	A
32	XA	536	C
32	XA	547	A
32	XA	559	A
32	XA	561	U
32	XA	564	C
32	XA	572	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
32	XA	573	A
32	XA	574	A
32	XA	575	G
32	XA	576	G
32	XA	577	G
32	XA	596	C
32	XA	630	G
32	XA	631	G
32	XA	632	A
32	XA	646	U
32	XA	653	A
32	XA	661	G
32	XA	665	A
32	XA	688	G
32	XA	695	A
32	XA	701	C
32	XA	721	G
32	XA	723	U
32	XA	724	G
32	XA	731	G
32	XA	749	C
32	XA	753	A
32	XA	755	G
32	XA	766	A
32	XA	774	G
32	XA	776	G
32	XA	777	A
32	XA	792	A
32	XA	793	U
32	XA	794	A
32	XA	816	A
32	XA	817	C
32	XA	818	G
32	XA	821	G
32	XA	828	A
32	XA	829	G
32	XA	836	G
32	XA	840	C
32	XA	841	U
32	XA	848	C
32	XA	851	G
32	XA	902	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
32	XA	914	A
32	XA	926	G
32	XA	927	G
32	XA	931	C
32	XA	934	C
32	XA	935	A
32	XA	960	U
32	XA	961	U
32	XA	965	A
32	XA	968	A
32	XA	969	A
32	XA	971	G
32	XA	974	A
32	XA	975	A
32	XA	976	G
32	XA	977	A
32	XA	992	U
32	XA	993	G
32	XA	994	A
32	XA	1003	G
32	XA	1004	A
32	XA	1005	A
32	XA	1006	C
32	XA	1009	G
32	XA	1016	A
32	XA	1020	U
32	XA	1022	G
32	XA	1023	G
32	XA	1025	U
32	XA	1026	G
32	XA	1027	C
32	XA	1028	C
32	XA	1030(B)	G
32	XA	1030(C)	C
32	XA	1038	C
32	XA	1041	A
32	XA	1043	C
32	XA	1044	A
32	XA	1045	C
32	XA	1065	U
32	XA	1066	C
32	XA	1068	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
32	XA	1081	G
32	XA	1094	G
32	XA	1095	U
32	XA	1101	A
32	XA	1117	G
32	XA	1125	U
32	XA	1129	C
32	XA	1130	A
32	XA	1136	U
32	XA	1137	C
32	XA	1139	G
32	XA	1147	C
32	XA	1152	A
32	XA	1159	U
32	XA	1160	G
32	XA	1183	A
32	XA	1184	G
32	XA	1196	U
32	XA	1197	G
32	XA	1211	U
32	XA	1213	A
32	XA	1227	A
32	XA	1236	A
32	XA	1238	A
32	XA	1250	A
32	XA	1256	A
32	XA	1257	U
32	XA	1258	G
32	XA	1270	C
32	XA	1278	U
32	XA	1279	A
32	XA	1280	A
32	XA	1281	U
32	XA	1282	C
32	XA	1286	A
32	XA	1287	A
32	XA	1300	G
32	XA	1302	U
32	XA	1305	G
32	XA	1320	C
32	XA	1329	A
32	XA	1340	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
32	XA	1346	A
32	XA	1347	G
32	XA	1353	G
32	XA	1363(A)	C
32	XA	1363(B)	A
32	XA	1364	U
32	XA	1397	C
32	XA	1401	G
32	XA	1419	G
32	XA	1442(A)	G
32	XA	1442(B)	G
32	XA	1447	A
32	XA	1456	G
32	XA	1457	G
32	XA	1487	G
32	XA	1491	G
32	XA	1493	A
32	XA	1497	G
32	XA	1503	A
32	XA	1504	G
32	XA	1507	A
32	XA	1517	G
32	XA	1520	G
32	XA	1525	G
32	XA	1529	G
32	XA	1530	G
53	XV	2	G
53	XV	4	G
53	XV	5	G
53	XV	8	U
53	XV	9	G
53	XV	17(A)	U
53	XV	18	G
53	XV	19	G
53	XV	21	A
53	XV	22	G
53	XV	31	G
53	XV	47	U
53	XV	48	C
53	XV	54	U
53	XV	68	C
53	XV	76	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
54	XX	15	A
54	XX	17	U
54	XX	21	A
54	XX	22	C

All (78) RNA pucker outliers are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	RA	9	U
1	RA	214	G
1	RA	272(M)	G
1	RA	277	C
1	RA	752	A
1	RA	856	C
1	RA	1045	A
1	RA	1053	C
1	RA	1057	A
1	RA	1065	U
1	RA	1067	A
1	RA	1073	A
1	RA	1210	A
1	RA	1240	U
1	RA	1420	U
1	RA	1530	C
1	RA	1992	G
1	RA	2126	A
1	RA	2171	A
1	RA	2172	U
1	RA	2321	G
1	RA	2689	U
32	QA	115	G
32	QA	266	G
32	QA	509	A
32	QA	560	U
32	QA	687	A
32	QA	839	U
32	QA	913	A
32	QA	943	U
32	QA	991	U
32	QA	1065	U
32	QA	1067	A
32	QA	1201	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
32	QA	1207	2MG
32	QA	1285	A
32	QA	1442(A)	G
1	YA	9	U
1	YA	272(M)	G
1	YA	277	C
1	YA	752	A
1	YA	764	A
1	YA	774	A
1	YA	827	U
1	YA	832	G
1	YA	958	U
1	YA	1053	C
1	YA	1057	A
1	YA	1065	U
1	YA	1067	A
1	YA	1073	A
1	YA	1420	U
1	YA	1530	C
1	YA	1608	A
1	YA	1992	G
1	YA	2126	A
1	YA	2171	A
1	YA	2172	U
1	YA	2321	G
1	YA	2430	A
1	YA	2689	U
32	XA	60	A
32	XA	115	G
32	XA	266	G
32	XA	509	A
32	XA	560	U
32	XA	687	A
32	XA	748	C
32	XA	840	C
32	XA	913	A
32	XA	991	U
32	XA	992	U
32	XA	1065	U
32	XA	1067	A
32	XA	1183	A
32	XA	1256	A

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Mol	Chain	Res	Type
32	XA	1442(A)	G
53	XV	53	G

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

48 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
1	5MC	YA	1942	1	18,22,23	3.71	6 (33%)	26,32,35	1.56	5 (19%)
32	2MG	XA	1207	32	18,26,27	2.84	6 (33%)	16,38,41	2.32	4 (25%)
1	OMG	YA	2251	53,56,1	18,26,27	2.74	7 (38%)	19,38,41	2.59	7 (36%)
32	5MC	QA	1404	32	18,22,23	3.91	6 (33%)	26,32,35	1.51	3 (11%)
1	2MU	YA	2552	56,1	19,22,24	6.01	13 (68%)	26,31,36	3.26	9 (34%)
32	5MC	QA	1407	32	18,22,23	3.88	6 (33%)	26,32,35	1.46	3 (11%)
32	MA6	QA	1518	32	19,26,27	1.27	2 (10%)	18,38,41	3.29	2 (11%)
32	MA6	QA	1519	32	19,26,27	1.28	3 (15%)	18,38,41	3.53	2 (11%)
1	PSU	YA	1917	1	18,21,22	0.96	1 (5%)	22,30,33	1.69	4 (18%)
32	M2G	QA	966	32	20,27,28	3.94	6 (30%)	22,40,43	1.84	5 (22%)
32	7MG	XA	527	56,32	22,26,27	5.95	10 (45%)	29,39,42	3.61	12 (41%)
32	4OC	QA	1402	32	20,23,24	3.23	7 (35%)	26,32,35	1.20	2 (7%)
1	PSU	YA	2605	1	18,21,22	1.01	1 (5%)	22,30,33	1.42	3 (13%)
1	2MU	RA	2552	56,1	19,22,24	5.97	12 (63%)	26,31,36	3.11	10 (38%)
32	5MC	QA	1400	32	18,22,23	3.82	6 (33%)	26,32,35	1.36	3 (11%)
32	UR3	QA	1498	32	19,22,23	3.09	6 (31%)	26,32,35	1.71	5 (19%)
1	PSU	YA	1911	1	18,21,22	1.06	1 (5%)	22,30,33	1.61	5 (22%)
32	5MC	XA	1404	32	18,22,23	3.79	6 (33%)	26,32,35	1.55	4 (15%)
32	5MC	XA	1407	32	18,22,23	3.94	6 (33%)	26,32,35	1.76	6 (23%)
1	5MU	RA	1939	1	19,22,23	4.79	5 (26%)	28,32,35	3.71	8 (28%)
1	PSU	RA	1911	1	18,21,22	1.01	1 (5%)	22,30,33	1.52	4 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
32	4OC	XA	1402	32	20,23,24	3.09	7 (35%)	26,32,35	1.34	4 (15%)
1	PSU	RA	2605	1	18,21,22	1.07	1 (5%)	22,30,33	1.82	3 (13%)
32	PSU	XA	516	32	18,21,22	1.02	1 (5%)	22,30,33	1.57	4 (18%)
32	UR3	XA	1498	56,32	19,22,23	3.03	6 (31%)	26,32,35	1.61	3 (11%)
1	PSU	RA	1917	1	18,21,22	1.07	1 (5%)	22,30,33	1.50	4 (18%)
32	7MG	QA	527	56,32	22,26,27	6.10	10 (45%)	29,39,42	3.77	12 (41%)
43	0TD	XL	92	43	7,9,10	1.14	0	6,11,13	2.67	4 (66%)
32	MA6	XA	1518	32	19,26,27	1.16	2 (10%)	18,38,41	3.42	2 (11%)
32	5MC	QA	967	32	18,22,23	3.92	6 (33%)	26,32,35	1.46	4 (15%)
32	2MG	QA	1207	32	18,26,27	2.92	6 (33%)	16,38,41	2.43	4 (25%)
1	4OC	YA	1920	1	19,22,24	3.10	7 (36%)	26,31,35	1.21	3 (11%)
1	5MC	YA	1962	56,1	18,22,23	3.57	6 (33%)	26,32,35	1.32	4 (15%)
32	5MC	XA	1400	32	18,22,23	3.85	6 (33%)	26,32,35	1.67	4 (15%)
1	4OC	RA	1920	1	19,22,24	3.26	7 (36%)	26,31,35	1.26	3 (11%)
1	5MU	YA	1915	1	19,22,23	5.14	6 (31%)	28,32,35	3.54	11 (39%)
1	5MU	YA	1939	56,1	19,22,23	4.86	5 (26%)	28,32,35	4.07	9 (32%)
32	PSU	QA	516	56,32	18,21,22	1.15	1 (5%)	22,30,33	1.49	5 (22%)
43	0TD	QL	92	43	7,9,10	1.21	0	6,11,13	3.24	4 (66%)
32	M2G	XA	966	32	20,27,28	3.74	6 (30%)	22,40,43	1.88	5 (22%)
32	5MC	XA	967	32	18,22,23	3.90	6 (33%)	26,32,35	1.54	5 (19%)
1	5MU	RA	1915	1	19,22,23	5.09	6 (31%)	28,32,35	3.43	10 (35%)
32	MA6	XA	1519	32	19,26,27	1.44	2 (10%)	18,38,41	4.11	2 (11%)
1	5MC	RA	1962	56,1	18,22,23	3.66	6 (33%)	26,32,35	1.27	3 (11%)
1	5MC	RA	1942	56,1	18,22,23	3.78	6 (33%)	26,32,35	1.32	3 (11%)
1	2MA	YA	2503	56,1	17,25,26	2.65	5 (29%)	17,37,40	2.35	4 (23%)
1	OMG	RA	2251	53,56,1	18,26,27	2.72	6 (33%)	19,38,41	2.71	6 (31%)
1	2MA	RA	2503	56,1	17,25,26	2.75	5 (29%)	17,37,40	2.33	4 (23%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	5MC	YA	1942	1	-	0/7/25/26	0/2/2/2
32	2MG	XA	1207	32	-	0/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMG	YA	2251	53,56,1	-	0/5/27/28	0/3/3/3
32	5MC	QA	1404	32	-	0/7/25/26	0/2/2/2
1	2MU	YA	2552	56,1	-	0/9/27/28	0/2/2/2
32	5MC	QA	1407	32	-	0/7/25/26	0/2/2/2
32	MA6	QA	1518	32	-	0/7/29/30	0/3/3/3
32	MA6	QA	1519	32	-	3/7/29/30	0/3/3/3
1	PSU	YA	1917	1	-	0/7/25/26	0/2/2/2
32	M2G	QA	966	32	-	0/7/29/30	0/3/3/3
32	7MG	XA	527	56,32	-	2/7/37/38	0/3/3/3
32	4OC	QA	1402	32	-	2/9/29/30	0/2/2/2
1	PSU	YA	2605	1	-	0/7/25/26	0/2/2/2
1	2MU	RA	2552	56,1	-	0/9/27/28	0/2/2/2
32	5MC	QA	1400	32	-	2/7/25/26	0/2/2/2
32	UR3	QA	1498	32	-	0/7/25/26	0/2/2/2
1	PSU	YA	1911	1	-	0/7/25/26	0/2/2/2
32	5MC	XA	1404	32	-	0/7/25/26	0/2/2/2
32	5MC	XA	1407	32	-	0/7/25/26	0/2/2/2
1	5MU	RA	1939	1	-	2/7/25/26	0/2/2/2
1	PSU	RA	1911	1	-	0/7/25/26	0/2/2/2
32	4OC	XA	1402	32	-	2/9/29/30	0/2/2/2
1	PSU	RA	2605	1	-	0/7/25/26	0/2/2/2
32	PSU	XA	516	32	-	0/7/25/26	0/2/2/2
32	UR3	XA	1498	56,32	-	0/7/25/26	0/2/2/2
1	PSU	RA	1917	1	-	0/7/25/26	0/2/2/2
32	7MG	QA	527	56,32	-	2/7/37/38	0/3/3/3
43	0TD	XL	92	43	-	3/7/12/14	-
32	MA6	XA	1518	32	-	1/7/29/30	0/3/3/3
32	5MC	QA	967	32	-	0/7/25/26	0/2/2/2
32	2MG	QA	1207	32	-	0/5/27/28	0/3/3/3
1	4OC	YA	1920	1	-	1/9/27/30	0/2/2/2
1	5MC	YA	1962	56,1	-	0/7/25/26	0/2/2/2
32	5MC	XA	1400	32	-	2/7/25/26	0/2/2/2
1	4OC	RA	1920	1	-	0/9/27/30	0/2/2/2
1	5MU	YA	1915	1	-	2/7/25/26	0/2/2/2
1	5MU	YA	1939	56,1	-	0/7/25/26	0/2/2/2
32	PSU	QA	516	56,32	-	0/7/25/26	0/2/2/2
43	0TD	QL	92	43	-	1/7/12/14	-
32	M2G	XA	966	32	-	0/7/29/30	0/3/3/3
32	5MC	XA	967	32	-	0/7/25/26	0/2/2/2
1	5MU	RA	1915	1	-	2/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	MA6	XA	1519	32	-	3/7/29/30	0/3/3/3
1	5MC	RA	1962	56,1	-	0/7/25/26	0/2/2/2
1	5MC	RA	1942	56,1	-	0/7/25/26	0/2/2/2
1	2MA	YA	2503	56,1	-	2/3/25/26	0/3/3/3
1	OMG	RA	2251	53,56,1	-	0/5/27/28	0/3/3/3
1	2MA	RA	2503	56,1	-	1/3/25/26	0/3/3/3

All (243) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	QA	527	7MG	C8-N9	19.67	1.56	1.46
32	XA	527	7MG	C8-N9	18.81	1.56	1.46
1	YA	2552	2MU	C5-C4	14.17	1.75	1.43
1	RA	2552	2MU	C5-C4	14.11	1.74	1.43
32	QA	966	M2G	C2-N3	13.73	1.47	1.30
32	XA	966	M2G	C2-N3	13.19	1.46	1.30
1	YA	1915	5MU	C6-N1	12.45	1.59	1.38
1	RA	1915	5MU	C6-N1	12.08	1.58	1.38
1	YA	1939	5MU	C6-N1	12.02	1.58	1.38
1	RA	1939	5MU	C6-N1	11.84	1.58	1.38
1	YA	1915	5MU	C2-N1	11.73	1.57	1.38
1	RA	1915	5MU	C2-N1	11.31	1.56	1.38
1	YA	2552	2MU	C4-N3	-11.03	1.18	1.38
1	YA	1939	5MU	C2-N1	10.81	1.55	1.38
1	RA	2552	2MU	C4-N3	-10.72	1.19	1.38
1	RA	1939	5MU	C2-N1	10.32	1.55	1.38
32	QA	527	7MG	C4-N9	10.28	1.49	1.37
32	XA	527	7MG	C5-N7	10.21	1.47	1.35
32	QA	527	7MG	C5-N7	9.89	1.47	1.35
32	XA	527	7MG	C4-N9	9.87	1.49	1.37
1	YA	2552	2MU	C6-N1	9.85	1.61	1.38
1	RA	1915	5MU	C4-C5	9.56	1.60	1.44
1	RA	2552	2MU	C6-N1	9.34	1.60	1.38
1	YA	1915	5MU	C4-C5	9.31	1.60	1.44
32	QA	1498	UR3	C2-N1	8.85	1.51	1.38
32	XA	1498	UR3	C2-N1	8.68	1.51	1.38
1	RA	1939	5MU	C4-C5	8.65	1.59	1.44
32	QA	1407	5MC	C6-C5	8.61	1.48	1.34
1	RA	2552	2MU	C3'-C2'	-8.52	1.34	1.52
32	QA	1400	5MC	C6-C5	8.51	1.48	1.34
32	XA	1400	5MC	C4-N3	8.49	1.48	1.34
32	QA	967	5MC	C6-C5	8.43	1.48	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	XA	1407	5MC	C6-C5	8.43	1.48	1.34
1	YA	1939	5MU	C4-C5	8.43	1.58	1.44
32	QA	1404	5MC	C6-C5	8.43	1.48	1.34
1	YA	2552	2MU	C3'-C2'	-8.39	1.34	1.52
32	QA	967	5MC	C4-N3	8.38	1.48	1.34
32	XA	967	5MC	C6-C5	8.37	1.48	1.34
32	XA	1404	5MC	C6-C5	8.33	1.48	1.34
1	YA	1962	5MC	C4-N3	8.31	1.48	1.34
32	XA	967	5MC	C4-N3	8.27	1.48	1.34
32	XA	1400	5MC	C6-C5	8.26	1.48	1.34
32	QA	1400	5MC	C4-N3	8.24	1.48	1.34
32	XA	1407	5MC	C4-N3	8.24	1.48	1.34
1	YA	1942	5MC	C6-C5	8.23	1.48	1.34
1	RA	1942	5MC	C6-C5	8.20	1.48	1.34
32	QA	1404	5MC	C4-N3	8.19	1.48	1.34
1	RA	1962	5MC	C6-C5	8.09	1.47	1.34
1	RA	1915	5MU	C6-C5	8.05	1.47	1.34
32	QA	1402	4OC	C4-N3	7.99	1.46	1.32
1	RA	2503	2MA	C2-N3	7.94	1.48	1.31
1	YA	1915	5MU	C6-C5	7.89	1.47	1.34
1	RA	1942	5MC	C4-N3	7.87	1.47	1.34
1	RA	1962	5MC	C4-N3	7.83	1.47	1.34
32	XA	1404	5MC	C4-N3	7.77	1.47	1.34
32	QA	1407	5MC	C4-N3	7.71	1.47	1.34
1	YA	1942	5MC	C4-N3	7.57	1.46	1.34
1	YA	1939	5MU	C4-N3	-7.53	1.24	1.38
1	RA	1939	5MU	C4-N3	-7.46	1.25	1.38
1	YA	1962	5MC	C6-C5	7.45	1.46	1.34
32	QA	966	M2G	C2-N2	7.41	1.49	1.35
1	YA	2503	2MA	C2-N3	7.39	1.46	1.31
32	XA	1400	5MC	C2-N3	7.19	1.50	1.36
1	RA	1939	5MU	C6-C5	7.14	1.46	1.34
32	QA	527	7MG	C4-N3	7.10	1.51	1.34
32	QA	527	7MG	C2-N3	7.10	1.50	1.33
32	XA	1407	5MC	C2-N3	7.10	1.50	1.36
1	YA	2552	2MU	O4'-C1'	7.09	1.58	1.42
1	RA	1915	5MU	C4-N3	-7.01	1.25	1.38
1	YA	1939	5MU	C6-C5	7.00	1.46	1.34
32	QA	1404	5MC	C2-N3	6.99	1.50	1.36
1	YA	1915	5MU	C4-N3	-6.99	1.25	1.38
32	XA	1402	4OC	C4-N3	6.95	1.44	1.32
32	XA	967	5MC	C2-N3	6.93	1.50	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	XA	527	7MG	C2-N3	6.92	1.49	1.33
32	QA	1400	5MC	C2-N3	6.91	1.50	1.36
1	RA	2552	2MU	O4'-C1'	6.89	1.58	1.42
32	QA	967	5MC	C2-N3	6.86	1.50	1.36
1	RA	1920	4OC	C6-C5	6.84	1.51	1.35
32	XA	966	M2G	C2-N2	6.82	1.48	1.35
32	XA	527	7MG	C4-N3	6.82	1.50	1.34
32	QA	1407	5MC	C2-N3	6.81	1.50	1.36
1	RA	1962	5MC	C2-N3	6.76	1.50	1.36
32	XA	1404	5MC	C2-N3	6.69	1.49	1.36
1	YA	1920	4OC	C6-C5	6.68	1.50	1.35
1	YA	1962	5MC	C2-N3	6.61	1.49	1.36
1	RA	1942	5MC	C2-N3	6.58	1.49	1.36
1	YA	1942	5MC	C2-N3	6.51	1.49	1.36
32	QA	1207	2MG	C2-N2	6.47	1.47	1.33
1	RA	2552	2MU	C6-C5	-6.43	1.20	1.35
32	XA	1402	4OC	C6-C5	6.43	1.50	1.35
32	QA	1402	4OC	C6-C5	6.40	1.49	1.35
32	XA	1207	2MG	C2-N1	6.40	1.46	1.36
32	QA	1207	2MG	C2-N1	6.37	1.46	1.36
1	YA	2552	2MU	C6-C5	-6.34	1.20	1.35
1	RA	1920	4OC	C2-N3	6.32	1.49	1.36
32	XA	1407	5MC	C6-N1	6.23	1.48	1.38
1	RA	1920	4OC	C4-N3	6.22	1.47	1.34
32	QA	527	7MG	C2-N2	6.14	1.48	1.34
32	XA	1207	2MG	C2-N2	6.14	1.47	1.33
32	QA	1407	5MC	C6-N1	6.12	1.48	1.38
1	RA	2552	2MU	O4'-C4'	-6.05	1.31	1.45
32	XA	527	7MG	C2-N2	6.02	1.48	1.34
32	QA	1404	5MC	C6-N1	6.01	1.48	1.38
1	YA	1920	4OC	C2-N3	5.99	1.48	1.36
32	QA	967	5MC	C6-N1	5.95	1.48	1.38
32	QA	1498	UR3	C2-N3	5.92	1.50	1.39
32	XA	1498	UR3	C2-N3	5.89	1.50	1.39
1	YA	2503	2MA	C4-N3	5.88	1.51	1.37
32	QA	1402	4OC	C2-N3	5.88	1.48	1.36
32	QA	1498	UR3	C6-C5	5.85	1.48	1.35
1	YA	1920	4OC	C4-N3	5.84	1.46	1.34
32	XA	967	5MC	C6-N1	5.84	1.48	1.38
32	XA	1498	UR3	C6-C5	5.83	1.48	1.35
1	RA	2503	2MA	C4-N3	5.80	1.51	1.37
32	XA	1404	5MC	C6-N1	5.73	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	YA	2552	2MU	O4'-C4'	-5.71	1.32	1.45
1	RA	1920	4OC	C4-N4	5.65	1.47	1.33
1	YA	2251	OMG	C2-N2	5.59	1.47	1.34
1	RA	2552	2MU	C1'-N1	-5.55	1.31	1.47
32	XA	527	7MG	C6-N1	5.53	1.49	1.38
1	YA	1942	5MC	C6-N1	5.51	1.47	1.38
1	RA	1942	5MC	C6-N1	5.49	1.47	1.38
1	YA	2251	OMG	C2-N3	5.49	1.46	1.33
1	YA	2552	2MU	C1'-N1	-5.49	1.31	1.47
32	QA	527	7MG	C6-N1	5.48	1.49	1.38
32	QA	1207	2MG	C6-N1	5.38	1.45	1.37
1	RA	2251	OMG	C2-N3	5.32	1.46	1.33
32	XA	1400	5MC	C6-N1	5.32	1.47	1.38
32	XA	1402	4OC	C2-N3	5.32	1.47	1.36
1	RA	2251	OMG	C2-N2	5.29	1.46	1.34
32	XA	1207	2MG	C6-N1	5.27	1.45	1.37
32	QA	1400	5MC	C6-N1	5.25	1.47	1.38
1	YA	1920	4OC	C4-N4	5.24	1.46	1.33
32	QA	1207	2MG	C4-N3	5.20	1.50	1.37
32	XA	1404	5MC	C4-N4	5.13	1.47	1.34
32	XA	527	7MG	C2-N1	5.11	1.50	1.37
32	QA	967	5MC	C4-N4	5.10	1.47	1.34
32	QA	1404	5MC	C4-N4	5.07	1.47	1.34
32	QA	527	7MG	C2-N1	5.06	1.50	1.37
32	XA	967	5MC	C4-N4	5.05	1.47	1.34
32	XA	1207	2MG	C4-N3	4.98	1.49	1.37
32	QA	1402	4OC	C4-N4	4.93	1.46	1.35
1	RA	1942	5MC	C2-N1	4.93	1.50	1.40
1	RA	1942	5MC	C4-N4	4.93	1.46	1.34
1	YA	1942	5MC	C4-N4	4.92	1.46	1.34
32	QA	1407	5MC	C4-N4	4.91	1.46	1.34
32	XA	1407	5MC	C4-N4	4.90	1.46	1.34
32	QA	966	M2G	C4-N3	4.86	1.49	1.37
1	RA	2251	OMG	C6-N1	4.83	1.45	1.37
1	RA	1962	5MC	C6-N1	4.81	1.46	1.38
32	XA	1400	5MC	C4-N4	4.77	1.46	1.34
32	QA	1407	5MC	C2-N1	4.75	1.50	1.40
32	XA	1402	4OC	C4-N4	4.73	1.45	1.35
32	XA	967	5MC	C2-N1	4.71	1.50	1.40
32	XA	1407	5MC	C2-N1	4.67	1.50	1.40
32	QA	1400	5MC	C4-N4	4.67	1.46	1.34
32	XA	966	M2G	C4-N3	4.64	1.48	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	RA	1962	5MC	C4-N4	4.56	1.46	1.34
32	QA	967	5MC	C2-N1	4.54	1.49	1.40
1	RA	1920	4OC	C2-N1	4.54	1.49	1.40
32	QA	1404	5MC	C2-N1	4.51	1.49	1.40
1	YA	1962	5MC	C4-N4	4.50	1.45	1.34
32	QA	966	M2G	C6-N1	4.43	1.44	1.37
32	QA	1400	5MC	C2-N1	4.40	1.49	1.40
1	RA	2251	OMG	C4-N3	4.39	1.48	1.37
1	YA	1962	5MC	C6-N1	4.38	1.45	1.38
1	RA	1962	5MC	C2-N1	4.34	1.49	1.40
1	YA	2251	OMG	C4-N3	4.34	1.47	1.37
1	YA	1942	5MC	C2-N1	4.33	1.49	1.40
32	XA	1400	5MC	C2-N1	4.25	1.49	1.40
32	XA	1404	5MC	C2-N1	4.23	1.49	1.40
32	XA	527	7MG	C5-C6	4.23	1.54	1.43
1	YA	1920	4OC	C2-N1	4.16	1.49	1.40
32	XA	1402	4OC	C2-N1	4.15	1.49	1.40
1	YA	1962	5MC	C2-N1	4.07	1.48	1.40
32	QA	1402	4OC	C5-C4	4.06	1.49	1.40
32	XA	966	M2G	C6-N1	4.05	1.43	1.37
32	XA	1402	4OC	C5-C4	4.02	1.49	1.40
1	RA	2552	2MU	C3'-C4'	4.00	1.63	1.53
32	QA	527	7MG	C5-C6	3.99	1.53	1.43
32	QA	1402	4OC	C2-N1	3.98	1.48	1.40
1	YA	2251	OMG	C6-N1	3.95	1.43	1.37
1	RA	2251	OMG	C2-N1	3.92	1.47	1.37
1	YA	2251	OMG	C2-N1	3.79	1.47	1.37
1	YA	2552	2MU	C3'-C4'	3.78	1.62	1.53
32	QA	516	PSU	C6-C5	3.77	1.39	1.35
1	RA	2503	2MA	C6-N1	3.65	1.46	1.38
1	YA	2251	OMG	O6-C6	-3.46	1.16	1.23
1	RA	1920	4OC	C6-N1	3.46	1.46	1.38
1	YA	2503	2MA	C6-N1	3.44	1.45	1.38
32	QA	966	M2G	C2-N1	3.43	1.45	1.36
1	YA	1911	PSU	C6-C5	3.42	1.39	1.35
1	RA	1917	PSU	C6-C5	3.39	1.39	1.35
1	RA	2251	OMG	O6-C6	-3.38	1.16	1.23
1	YA	1920	4OC	C6-N1	3.31	1.46	1.38
32	QA	1519	MA6	C2-N3	3.31	1.37	1.32
32	XA	1402	4OC	C6-N1	3.30	1.46	1.38
32	QA	1498	UR3	C4-N3	3.30	1.48	1.40
32	XA	1519	MA6	C10-N6	3.28	1.53	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	QA	1498	UR3	C6-N1	3.19	1.45	1.38
1	RA	1911	PSU	C6-C5	3.19	1.39	1.35
32	XA	966	M2G	C2-N1	3.19	1.44	1.36
1	YA	2605	PSU	C6-C5	3.15	1.39	1.35
32	XA	1498	UR3	C6-N1	3.14	1.45	1.38
32	XA	516	PSU	C6-C5	3.12	1.39	1.35
32	QA	1402	4OC	C6-N1	3.11	1.45	1.38
1	RA	2605	PSU	C6-C5	3.10	1.38	1.35
1	YA	1917	PSU	C6-C5	3.03	1.38	1.35
1	RA	1920	4OC	C5-C4	3.01	1.49	1.42
32	XA	1498	UR3	C4-N3	2.98	1.47	1.40
1	YA	2552	2MU	C2-N1	2.91	1.43	1.38
1	RA	2552	2MU	C2-N1	2.89	1.43	1.38
32	XA	527	7MG	C5-C4	2.85	1.47	1.38
32	QA	527	7MG	C5-C4	2.78	1.47	1.38
1	YA	2552	2MU	O2-C2	-2.78	1.18	1.23
32	XA	1518	MA6	C2-N3	2.75	1.36	1.32
32	XA	1519	MA6	C2-N3	2.74	1.36	1.32
1	YA	1920	4OC	C5-C4	2.72	1.49	1.42
32	QA	1498	UR3	C5-C4	2.61	1.50	1.43
32	XA	1498	UR3	C5-C4	2.56	1.50	1.43
32	QA	1518	MA6	C2-N3	2.55	1.36	1.32
1	RA	2503	2MA	CM2-C2	2.53	1.56	1.49
1	RA	2503	2MA	C2-N1	2.48	1.44	1.36
1	YA	2251	OMG	C5-C6	2.46	1.52	1.47
32	QA	1518	MA6	C2-N1	2.41	1.38	1.33
1	RA	2552	2MU	O2-C2	-2.37	1.18	1.23
1	YA	2503	2MA	CM2-C2	2.32	1.55	1.49
1	RA	2552	2MU	O2'-C2'	2.32	1.48	1.42
32	XA	1207	2MG	C5-C6	2.27	1.52	1.47
1	YA	2503	2MA	C2-N1	2.19	1.43	1.36
1	RA	1915	5MU	O2-C2	-2.18	1.19	1.23
32	QA	1207	2MG	C5-C6	2.16	1.51	1.47
32	XA	966	M2G	C5-C6	2.13	1.51	1.47
1	YA	2552	2MU	O2'-C2'	2.13	1.48	1.42
32	QA	966	M2G	C5-C6	2.12	1.51	1.47
1	YA	1915	5MU	C5M-C5	2.11	1.55	1.50
32	QA	1207	2MG	C5-C4	-2.08	1.37	1.43
32	XA	1518	MA6	C2-N1	2.07	1.37	1.33
32	XA	1207	2MG	C5-C4	-2.05	1.37	1.43
32	QA	1519	MA6	C5-C4	-2.05	1.35	1.40
32	QA	1519	MA6	C10-N6	2.03	1.50	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	YA	2552	2MU	O4-C4	-2.00	1.20	1.24

All (235) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	XA	1519	MA6	N1-C6-N6	-16.79	99.39	117.06
1	YA	1939	5MU	C5-C4-N3	14.60	127.77	115.31
32	QA	1519	MA6	N1-C6-N6	-13.43	102.92	117.06
1	RA	1939	5MU	C5-C4-N3	13.26	126.63	115.31
32	XA	1518	MA6	N1-C6-N6	-13.13	103.24	117.06
1	YA	1915	5MU	C5-C4-N3	12.55	126.02	115.31
32	QA	1518	MA6	N1-C6-N6	-12.19	104.22	117.06
1	YA	1939	5MU	C5-C6-N1	-11.82	111.17	123.34
1	RA	1939	5MU	C5-C6-N1	-11.26	111.76	123.34
1	RA	1915	5MU	C5-C4-N3	10.71	124.45	115.31
32	QA	527	7MG	C2-N3-C4	9.54	129.31	112.30
1	YA	2552	2MU	C5-C4-N3	9.50	129.05	114.84
32	XA	527	7MG	C2-N3-C4	9.37	129.00	112.30
1	RA	2552	2MU	C5-C4-N3	9.30	128.75	114.84
32	QA	527	7MG	C5-C6-N1	8.88	126.65	110.99
32	XA	527	7MG	C5-C6-N1	8.46	125.89	110.99
1	YA	1915	5MU	C5-C6-N1	-8.08	115.03	123.34
1	YA	2552	2MU	O4-C4-N3	-8.00	107.56	119.31
1	RA	1915	5MU	C5-C6-N1	-7.83	115.28	123.34
1	RA	2503	2MA	C5-C6-N1	7.26	126.55	114.02
1	YA	2503	2MA	C5-C6-N1	7.18	126.41	114.02
1	RA	2552	2MU	O4-C4-N3	-6.98	109.05	119.31
32	QA	1207	2MG	C5-C6-N1	6.58	125.57	113.95
1	RA	2552	2MU	C4-N3-C2	-6.54	117.95	126.58
32	QA	527	7MG	O6-C6-C5	-6.46	111.69	127.54
32	XA	1207	2MG	C5-C6-N1	6.38	125.22	113.95
1	RA	2251	OMG	C5-C6-N1	6.28	125.05	113.95
32	QA	527	7MG	N1-C2-N3	-6.26	111.63	123.32
32	QA	1498	UR3	C4-N3-C2	-6.26	118.67	124.56
1	YA	1939	5MU	O4-C4-N3	-6.22	108.19	120.12
1	YA	2251	OMG	C5-C6-N1	6.19	124.88	113.95
32	QA	1518	MA6	N3-C2-N1	-6.05	119.22	128.68
32	QA	1519	MA6	N3-C2-N1	-6.04	119.24	128.68
32	XA	527	7MG	N1-C2-N3	-6.01	112.10	123.32
32	XA	527	7MG	O6-C6-C5	-5.96	112.92	127.54
1	YA	2552	2MU	C4-N3-C2	-5.86	118.85	126.58
32	QA	527	7MG	C4-C5-N7	5.75	113.52	105.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	XA	1498	UR3	C4-N3-C2	-5.73	119.17	124.56
32	XA	1518	MA6	N3-C2-N1	-5.68	119.80	128.68
1	YA	1915	5MU	O4-C4-N3	-5.60	109.38	120.12
1	RA	1939	5MU	O4-C4-N3	-5.56	109.46	120.12
1	RA	2251	OMG	O6-C6-C5	-5.28	114.05	124.37
32	XA	1404	5MC	C5-C4-N3	-5.26	116.00	121.67
32	XA	527	7MG	C4-C5-N7	5.23	112.79	105.53
1	YA	2251	OMG	N1-C2-N3	-5.18	113.63	123.32
1	RA	2251	OMG	N1-C2-N3	-5.15	113.69	123.32
32	QA	527	7MG	C5-C4-N3	-5.09	118.43	128.13
32	QA	1207	2MG	O6-C6-C5	-5.08	114.45	124.37
1	RA	1915	5MU	O4-C4-N3	-5.01	110.50	120.12
1	RA	2605	PSU	N1-C2-N3	4.96	120.75	115.13
32	XA	527	7MG	C5-C4-N3	-4.95	118.70	128.13
1	YA	1942	5MC	C5-C4-N3	-4.86	116.43	121.67
1	RA	1915	5MU	N3-C2-N1	4.86	121.34	114.89
32	QA	527	7MG	N9-C8-N7	4.79	110.23	103.38
32	XA	966	M2G	C5-C6-N1	4.79	122.42	113.95
32	QA	527	7MG	N9-C4-N3	4.78	132.62	125.47
32	XA	527	7MG	N2-C2-N1	4.74	126.81	116.71
32	XA	1207	2MG	O6-C6-C5	-4.74	115.11	124.37
1	RA	1915	5MU	C5M-C5-C4	4.70	123.94	118.77
32	QA	527	7MG	N2-C2-N1	4.68	126.68	116.71
43	QL	92	0TD	CSB-SB-CB	4.65	110.86	102.44
1	RA	2251	OMG	N2-C2-N1	4.64	126.60	116.71
43	XL	92	0TD	CSB-SB-CB	4.55	110.67	102.44
32	QA	966	M2G	N1-C2-N2	4.49	121.86	118.04
32	QA	966	M2G	C5-C6-N1	4.49	121.87	113.95
32	XA	527	7MG	N9-C4-N3	4.47	132.16	125.47
32	XA	527	7MG	N9-C8-N7	4.45	109.74	103.38
32	QA	1404	5MC	C5-C4-N3	-4.44	116.88	121.67
1	YA	1917	PSU	C4-N3-C2	-4.42	119.97	126.34
32	XA	1407	5MC	C5-C4-N3	-4.38	116.95	121.67
1	YA	1915	5MU	C5M-C5-C4	4.35	123.56	118.77
32	XA	1400	5MC	C5-C4-N3	-4.34	116.99	121.67
32	QA	527	7MG	C6-C5-C4	-4.34	113.67	122.62
1	YA	2552	2MU	C6-C5-C4	-4.33	113.60	119.52
32	XA	1402	4OC	CM4-N4-C4	-4.29	114.07	122.45
43	QL	92	0TD	CB-CA-N	-4.27	100.00	109.10
32	QA	1407	5MC	C5-C4-N3	-4.25	117.08	121.67
1	RA	2605	PSU	C4-N3-C2	-4.24	120.22	126.34
32	XA	527	7MG	C6-C5-C4	-4.23	113.90	122.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	XA	967	5MC	C5-C4-N3	-4.22	117.12	121.67
1	RA	2503	2MA	N1-C2-N3	-4.17	116.14	123.06
32	QA	967	5MC	C5-C4-N3	-4.17	117.18	121.67
1	RA	1915	5MU	O2-C2-N3	-4.14	113.80	121.50
32	XA	1407	5MC	C4-N3-C2	4.13	126.27	120.69
1	YA	1917	PSU	N1-C2-N3	4.12	119.80	115.13
32	XA	516	PSU	C4-N3-C2	-4.07	120.48	126.34
1	YA	1915	5MU	O2-C2-N3	-4.06	113.93	121.50
1	YA	1939	5MU	C5M-C5-C4	4.03	123.20	118.77
1	YA	2503	2MA	N1-C2-N3	-4.02	116.40	123.06
1	RA	1911	PSU	C4-N3-C2	-4.01	120.56	126.34
1	YA	2251	OMG	C8-N7-C5	4.00	110.61	102.99
1	YA	1939	5MU	C4-N3-C2	-3.94	122.25	127.35
1	RA	1915	5MU	C5M-C5-C6	-3.94	117.59	122.85
32	QA	1404	5MC	C4-N3-C2	3.91	125.97	120.69
1	YA	2251	OMG	N2-C2-N1	3.90	125.02	116.71
1	RA	1915	5MU	C6-N1-C2	-3.89	117.36	121.30
32	XA	1400	5MC	C4-N3-C2	3.88	125.93	120.69
32	QA	1400	5MC	C5-C4-N3	-3.87	117.50	121.67
43	QL	92	0TD	OD2-CG-CB	3.87	121.51	113.15
1	YA	2605	PSU	C4-N3-C2	-3.87	120.77	126.34
32	XA	1404	5MC	C4-N3-C2	3.82	125.85	120.69
32	XA	966	M2G	N1-C2-N2	3.81	121.28	118.04
32	QA	1207	2MG	C8-N7-C5	3.81	110.24	102.99
32	XA	966	M2G	O6-C6-C5	-3.80	116.95	124.37
32	XA	1207	2MG	C8-N7-C5	3.80	110.22	102.99
1	RA	1911	PSU	N1-C2-N3	3.76	119.39	115.13
1	RA	2552	2MU	C6-C5-C4	-3.76	114.37	119.52
32	XA	1519	MA6	N3-C2-N1	-3.74	122.83	128.68
32	QA	1407	5MC	C4-N3-C2	3.73	125.73	120.69
1	YA	1911	PSU	N1-C2-N3	3.72	119.34	115.13
32	XA	967	5MC	C4-N3-C2	3.68	125.66	120.69
1	YA	1911	PSU	C4-N3-C2	-3.68	121.04	126.34
1	RA	1942	5MC	C5-C4-N3	-3.63	117.76	121.67
1	RA	1917	PSU	N1-C2-N3	3.61	119.22	115.13
1	RA	1915	5MU	C1'-N1-C2	3.61	124.10	117.57
32	QA	967	5MC	C4-N3-C2	3.59	125.54	120.69
32	QA	516	PSU	C4-N3-C2	-3.58	121.17	126.34
1	RA	1917	PSU	C4-N3-C2	-3.57	121.20	126.34
32	XA	1407	5MC	N4-C4-N3	3.55	124.96	118.48
32	QA	966	M2G	C8-N7-C5	3.54	109.74	102.99
1	YA	2552	2MU	O2-C2-N1	3.51	127.46	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	YA	2552	2MU	O2-C2-N3	-3.51	114.97	121.50
1	RA	1962	5MC	C5-C4-N3	-3.47	117.94	121.67
1	RA	2251	OMG	C8-N7-C5	3.46	109.59	102.99
1	RA	1939	5MU	C5M-C5-C4	3.46	122.58	118.77
1	YA	1915	5MU	N3-C2-N1	3.45	119.46	114.89
1	RA	1942	5MC	C4-N3-C2	3.41	125.30	120.69
1	RA	1939	5MU	C4-N3-C2	-3.41	122.94	127.35
32	XA	966	M2G	C8-N7-C5	3.38	109.43	102.99
1	YA	2251	OMG	O6-C6-C5	-3.35	117.82	124.37
1	YA	1942	5MC	C4-N3-C2	3.34	125.20	120.69
1	RA	1915	5MU	C4-N3-C2	-3.28	123.10	127.35
32	XA	1498	UR3	C6-N1-C2	-3.28	118.85	121.79
1	YA	1962	5MC	N4-C4-N3	3.27	124.45	118.48
32	QA	1400	5MC	C4-N3-C2	3.26	125.09	120.69
32	QA	516	PSU	N1-C2-N3	3.25	118.81	115.13
32	QA	966	M2G	O6-C6-C5	-3.24	118.04	124.37
1	YA	1939	5MU	C5M-C5-C6	-3.23	118.53	122.85
1	YA	2503	2MA	CM2-C2-N1	3.17	123.27	116.23
32	QA	1402	4OC	C5-C4-N3	-3.16	117.50	122.59
1	YA	1911	PSU	O2-C2-N1	-3.16	119.31	122.79
1	YA	1915	5MU	C1'-N1-C2	3.16	123.28	117.57
1	RA	2503	2MA	C8-N7-C5	3.15	109.00	102.99
32	XA	1400	5MC	N4-C4-N3	3.15	124.22	118.48
43	XL	92	0TD	OD2-CG-CB	3.14	119.93	113.15
1	YA	2503	2MA	C8-N7-C5	3.12	108.93	102.99
1	RA	2552	2MU	C5-C6-N1	-3.11	116.60	121.81
32	XA	967	5MC	N4-C4-N3	3.07	124.07	118.48
32	XA	966	M2G	C2-N1-C6	-3.03	118.68	123.71
32	XA	516	PSU	O2-C2-N1	-3.03	119.46	122.79
1	YA	1915	5MU	C4-N3-C2	-3.01	123.45	127.35
1	YA	1962	5MC	C5-C4-N4	-3.00	117.00	121.48
1	YA	2552	2MU	C5-C6-N1	-2.99	116.81	121.81
32	XA	516	PSU	N1-C2-N3	2.98	118.51	115.13
1	YA	2605	PSU	N1-C2-N3	2.98	118.50	115.13
1	YA	1962	5MC	C5-C4-N3	-2.89	118.55	121.67
1	RA	1939	5MU	C5M-C5-C6	-2.88	119.00	122.85
1	RA	1920	4OC	C5-C4-N3	-2.88	116.44	121.33
1	YA	1915	5MU	O2-C2-N1	2.87	126.60	122.79
1	RA	2552	2MU	O2-C2-N3	-2.85	116.19	121.50
1	RA	2503	2MA	CM2-C2-N1	2.85	122.56	116.23
1	YA	2251	OMG	O6-C6-N1	-2.84	117.30	120.65
1	RA	2605	PSU	C6-N1-C2	-2.83	119.79	122.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	YA	1917	PSU	O2-C2-N1	-2.81	119.70	122.79
32	QA	1402	4OC	C4-N3-C2	2.81	123.94	120.12
1	RA	2251	OMG	C2-N1-C6	-2.79	119.97	125.10
32	QA	967	5MC	N4-C4-N3	2.77	123.53	118.48
1	YA	1915	5MU	C5M-C5-C6	-2.75	119.17	122.85
1	YA	1942	5MC	C6-N1-C2	-2.73	117.09	120.87
1	RA	1920	4OC	C4-N3-C2	2.70	124.62	120.25
1	YA	1939	5MU	O2-C2-N3	-2.70	116.48	121.50
1	RA	1962	5MC	C4-N3-C2	2.66	124.29	120.69
1	YA	1920	4OC	N4-C4-N3	2.65	122.62	117.97
1	RA	1920	4OC	N4-C4-N3	2.64	122.59	117.97
1	RA	1917	PSU	O2-C2-N1	-2.64	119.89	122.79
32	XA	1407	5MC	C6-N1-C2	-2.63	117.23	120.87
32	QA	516	PSU	O2-C2-N1	-2.63	119.90	122.79
32	QA	527	7MG	C2-N1-C6	-2.63	120.31	125.10
1	YA	2251	OMG	C2-N1-C6	-2.62	120.27	125.10
32	XA	516	PSU	O4-C4-C5	-2.61	117.21	124.05
1	RA	1962	5MC	N4-C4-N3	2.59	123.20	118.48
32	QA	1498	UR3	C3U-N3-C4	2.59	121.59	117.89
32	XA	527	7MG	C2-N1-C6	-2.57	120.42	125.10
1	YA	1920	4OC	C5-C4-N3	-2.56	116.97	121.33
32	QA	1407	5MC	C6-N1-C2	-2.55	117.34	120.87
32	XA	1407	5MC	C5-C6-N1	2.54	125.96	123.34
1	YA	1911	PSU	C6-N1-C2	-2.52	120.11	122.68
1	YA	1915	5MU	C6-N1-C2	-2.51	118.76	121.30
32	QA	1498	UR3	C1'-N1-C2	2.49	121.19	116.99
1	RA	1917	PSU	C6-N1-C2	-2.48	120.15	122.68
1	YA	1920	4OC	C4-N3-C2	2.47	124.25	120.25
1	YA	1942	5MC	N4-C4-N3	2.45	122.95	118.48
1	RA	2552	2MU	N3-C2-N1	2.45	118.14	114.89
1	RA	1942	5MC	N4-C4-N3	2.45	122.94	118.48
1	RA	2552	2MU	C6-N1-C2	2.45	124.13	120.99
1	YA	2552	2MU	C6-N1-C2	2.45	124.12	120.99
32	XA	1400	5MC	C5-C6-N1	2.41	125.81	123.34
32	XA	1404	5MC	CM5-C5-C6	-2.39	119.66	122.85
32	QA	1400	5MC	N4-C4-N3	2.36	122.78	118.48
32	QA	1498	UR3	C6-N1-C2	-2.33	119.70	121.79
1	RA	1939	5MU	N3-C2-N1	2.31	117.96	114.89
32	QA	1404	5MC	N4-C4-N3	2.28	122.63	118.48
32	XA	1498	UR3	C1'-N1-C2	2.28	120.83	116.99
32	XA	1407	5MC	C5-C4-N4	-2.26	118.09	121.48
43	XL	92	0TD	CB-CA-N	-2.26	104.28	109.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	XA	967	5MC	C6-N1-C2	-2.26	117.75	120.87
1	YA	1942	5MC	CM5-C5-C6	-2.22	119.88	122.85
1	YA	1939	5MU	N3-C2-N1	2.21	117.82	114.89
1	YA	1939	5MU	O2-C2-N1	2.19	125.70	122.79
32	QA	966	M2G	C2-N1-C6	-2.19	120.08	123.71
32	XA	527	7MG	C5-C4-N9	2.16	109.15	106.35
1	RA	2552	2MU	O2-C2-N1	2.13	125.62	122.79
32	QA	516	PSU	C6-N1-C2	-2.11	120.53	122.68
1	RA	1911	PSU	C6-N1-C2	-2.11	120.53	122.68
32	XA	1402	4OC	O2-C2-N3	-2.10	118.91	122.33
32	QA	1207	2MG	O3'-C3'-C2'	2.10	118.60	111.82
32	XA	1402	4OC	C6-C5-C4	2.09	119.52	116.96
32	XA	1404	5MC	C6-N1-C2	-2.09	117.98	120.87
1	YA	2605	PSU	O2-C2-N1	-2.09	120.49	122.79
32	XA	1402	4OC	C5-C4-N3	-2.07	119.27	122.59
43	XL	92	0TD	OD2-CG-OD1	-2.06	119.42	124.09
1	RA	2552	2MU	C1'-N1-C2	-2.06	113.85	117.57
32	QA	516	PSU	O4-C4-C5	-2.04	118.70	124.05
32	QA	967	5MC	C6-N1-C2	-2.04	118.05	120.87
1	YA	1962	5MC	C4-N3-C2	2.03	123.44	120.69
1	RA	1911	PSU	O2-C2-N1	-2.03	120.55	122.79
1	YA	1917	PSU	C6-N1-C2	-2.03	120.61	122.68
1	RA	1939	5MU	O2-C2-N3	-2.02	117.73	121.50
32	XA	967	5MC	C5-C6-N1	2.02	125.42	123.34
32	QA	1498	UR3	O4-C4-C5	-2.01	118.33	124.37
1	YA	2552	2MU	N3-C2-N1	2.01	117.55	114.89
43	QL	92	0TD	OD2-CG-OD1	-2.00	119.54	124.09
1	YA	1911	PSU	O4-C4-C5	-2.00	118.81	124.05
32	XA	1207	2MG	CM2-N2-C2	-2.00	119.44	123.86
32	QA	527	7MG	C5-C4-N9	2.00	108.94	106.35

There are no chirality outliers.

All (33) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	RA	1915	5MU	O4'-C1'-N1-C2
1	RA	1915	5MU	O4'-C1'-N1-C6
32	QA	527	7MG	C3'-C4'-C5'-O5'
32	QA	1402	4OC	O4'-C4'-C5'-O5'
32	QA	1519	MA6	O4'-C4'-C5'-O5'
32	QA	1519	MA6	C5-C6-N6-C9
1	YA	1915	5MU	O4'-C1'-N1-C2

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Mol	Chain	Res	Type	Atoms
1	YA	1915	5MU	O4'-C1'-N1-C6
32	XA	1402	4OC	O4'-C4'-C5'-O5'
32	XA	1402	4OC	C3'-C4'-C5'-O5'
32	XA	1519	MA6	O4'-C4'-C5'-O5'
43	XL	92	0TD	O-C-CA-CB
43	XL	92	0TD	CG-CB-SB-CSB
1	RA	1939	5MU	O4'-C4'-C5'-O5'
32	QA	1402	4OC	C3'-C4'-C5'-O5'
32	QA	1519	MA6	C3'-C4'-C5'-O5'
32	XA	527	7MG	C3'-C4'-C5'-O5'
32	XA	1519	MA6	C3'-C4'-C5'-O5'
1	RA	1939	5MU	C3'-C4'-C5'-O5'
32	QA	527	7MG	O4'-C4'-C5'-O5'
32	QA	1400	5MC	O4'-C4'-C5'-O5'
32	QA	1400	5MC	C3'-C4'-C5'-O5'
32	XA	527	7MG	O4'-C4'-C5'-O5'
32	XA	1518	MA6	C5-C6-N6-C9
43	QL	92	0TD	CG-CB-SB-CSB
43	XL	92	0TD	SB-CB-CG-OD1
32	XA	1519	MA6	C5-C6-N6-C9
32	XA	1400	5MC	O4'-C4'-C5'-O5'
32	XA	1400	5MC	C3'-C4'-C5'-O5'
1	YA	1920	4OC	C2'-C1'-N1-C2
1	RA	2503	2MA	O4'-C4'-C5'-O5'
1	YA	2503	2MA	O4'-C4'-C5'-O5'
1	YA	2503	2MA	C4'-C5'-O5'-P

There are no ring outliers.

16 monomers are involved in 27 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	YA	2251	OMG	1	0
1	YA	2552	2MU	3	0
32	QA	1518	MA6	1	0
32	QA	1519	MA6	2	0
32	QA	1402	4OC	1	0
1	RA	2552	2MU	3	0
1	RA	1917	PSU	1	0
32	XA	1518	MA6	5	0
1	YA	1962	5MC	2	0
1	RA	1920	4OC	1	0
1	YA	1939	5MU	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	XA	1519	MA6	4	0
1	RA	1962	5MC	1	0
1	RA	1942	5MC	1	0
1	RA	2251	OMG	1	0
1	RA	2503	2MA	2	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 2450 ligands modelled in this entry, 2448 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
58	SF4	QD	302	35	0,12,12	-	-	-		
58	SF4	XD	301	35	0,12,12	-	-	-		

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
58	SF4	QD	302	35	-	-	0/6/5/5
58	SF4	XD	301	35	-	-	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

EDS failed to run properly - this section is therefore empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

EDS failed to run properly - this section is therefore empty.

### 6.3 Carbohydrates [i](#)

EDS failed to run properly - this section is therefore empty.

### 6.4 Ligands [i](#)

EDS failed to run properly - this section is therefore empty.

### 6.5 Other polymers [i](#)

EDS failed to run properly - this section is therefore empty.